Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

MASTER INDEX

VOLUMES 251-260

JANUARY-OCTOBER 2000

Editors
ROBIN M. HOCHSTRASSER
G. LUDWIG HOFACKER
H. PETER TROMMSDORFF

www.elsevier.nl/locate/chemphys

NORTH-HOLLAND

Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER

Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA Fax: 1-215-8980590; E-mail: hochstra@a.chem.upenn.edu

G. LUDWIG HOFACKER

Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany Fax: 49-89-28913622; E-mail: hofacker@theochem.tu-muenchen.de

H. PETER TROMMSDORFF

Laboratoire de Spectrométrie Physique, Université Joseph Fourier de Grenoble - CNRS, B.P. 87, 38402 Saint-Martin-d'Hères Cedex, France Fax: 33-476-514335; E-mail: chemphys@ujf-grenoble.fr

ASSOCIATE EDITOR

DAVID CHANDLER

Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA Fax: 1-510-6428369; E-mail: chandler@cchem.berkeley.edu

FOUNDING EDITORS: G.L. HOFACKER, G.W. ROBINSON, E.W. SCHLAG

Sweden

R. RIGLER, Stockholm

ADVISORY EDITORIAL BOARD

Australia	Hungary	Switzerland	USA (continued)
D.J. EVANS, Canberra	P. ORMOS, Szeged	H. FISCHER, Zurich	R.A. FRIESNER, New York, NY
N.S. HUSH, Sydney		S. LEUTWYLER, Bern	M. KLEIN, Philadelphia, PA
R.O. WATTS, Melbourne	Israel		W.C. LINEBERGER, Boulder, CO
	R.B. GERBER, Jerusalem	Taiwan	D.S. McCLURE, Princeton, NJ
Canada	J. JORTNER, Tel Aviv	Y.T. LEE, Taipei	D.M. NEUMARK, Berkeley, CA
R.J.D. MILLER, Toronto	R.D. LEVINE, Jerusalem	1.1. LEE, Taiper	M.D. NEWTON, Upton, NY
	E. POLLAK, Rehovot		C.S. PARMENTER,
Denmark		United Kingdom	Bloomington, IN
G.D. BILLING, Copenhagen	Italy	A.D. BUCKINGHAM, Cambridge	M.A. RATNER, Evanston, IL
-	G. CICCOTTI. Rome	D.C. CLARY, London	G.W. ROBINSON, Lubbock, TX
France	G. CICCOTTI, Rome	D.A. KING, Cambridge	G.J. SMALL, Ames, IA
S. LEACH, Meudon		P.A. MADDEN, Oxford	J.C. TULLY, New Haven, CT
D. MARKOVITSI, Gif-sur-Yvette	Japan	J.P. SIMONS, Oxford	J.D. WEEKS, College Park, MD
J.L. MARTIN, Palaiseau	H. HAMAGUCHI, Tokyo		K.B. WHALEY, Berkeley, CA
M. ORRIT, Talence	M. ITO, Okazaki	*10.4	P.G. WOLYNES, Urbana, IL
	T. KITAGAWA, Okazaki	USA	R.N. ZARE, Stanford, CA
Germany	T. KOBAYASHI, Tokyo	A.C. ALBRECHT, Ithaca, NY	A.H. ZEWAIL, Pasadena, CA
H. BÄSSLER, Marburg	K. YOSHIHARA, Ishikawa	P. ALIVISATOS, Berkeley, CA	
B.DICK, Regensburg		V.A. APKARIAN, Irvine, CA	
S.F. FISCHER, Garching	The Netherlands	P.F. BARBARA, Austin, TX	
H. GRABERT, Freiburg	D. FRENKEL, Amsterdam	R. BERSOHN, New York, NY	
D. HAARER, Bayreuth		S.G. BOXER, Stanford, CA	
P. HÄNGGI, Augsburg	Russian Federation	S.T. CEYER, Cambridge, MA	
W. LORENZ, Leipzig	V.S. LETOKHOV, Moscow	K.A. DILL, San Francisco, CA	
D. MENZEL, Garching		W.A. EATON, Bethesda, MD	
M. PARRINELLO, Stuttgart		M.D. FAYER, Stanford, CA	

W. ZINTH, Munich AIMS AND SCOPE

E.W. SCHLAG, Garching

Chemical Physics publishes experimental and theoretical papers on all aspects of chemical physics. Experimental papers are brought into relation with theory and theoretical papers demonstrate their relation to present or future experiments. More specifically, subject matter in the fields of spectroscopy and molecular structure, interacting systems, relaxation phenomena, fundamental problems in molecular reactivity, molecular quantum theory and statistical mechanics constitute the main areas of interest for this journal. In addition to regular issues, Chemical Physics publishes thematic issues containing invited articles by specialists in the relevant field.

G.R. FLEMING, Berkeley, CA

G. FLYNN, New York, NY

Chemical Physics

EDITORS

ROBIN M. HOCHSTRASSER

Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA Fax: 1-215-8980590; E-mail: hochstra@a.chem.upenn.edu

G. LUDWIG HOFACKER

Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany Fax; 49-89-28913622; E-mail: hofacker@theochem.tu-muenchen.de

H. PETER TROMMSDORFF

Laboratoire de Spectrométrie Physique, Université Joseph Fourier de Grenoble - CNRS, B.P. 87, 38402 Saint-Martin-d'Hères Cedex, France Fax: 33-476-514335; E-mail: chemphys@ujf-grenoble.fr

ASSOCIATE EDITOR

DAVID CHANDLER

Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA Fax: 1-510-6428369; E-mail: chandler@cchem.berkeley.edu

FOUNDING EDITORS: G.L. HOFACKER, G.W. ROBINSON, E.W. SCHLAG

ADVISORY EDITORIAL BOARD

Australia
D.J. EVANS, Canberra
N.S. HUSH, Sydney
R.O. WATTS, Melbourne

Canada

R.J.D. MILLER, Toronto

Denmark
G.D. BILLING, Copenhagen

France
S. LEACH, Meudon
D. MARKOVITSI, Gif-sur-Yvette
II MARTIN Palaiseau

D. MARKOVITSI, Gif-sur-Yve J.L. MARTIN, Palaiseau M. ORRIT, Talence

Germany
H. BÄSSLER, Marburg
B. DICK, Regensburg
S.F. FISCHER, Garching
H. GRABERT, Freiburg
D. HAARER, Bayreuth
P. HÄNGGI, Augsburg
W. LORENZ, Leipzig
D. MENZEL, Garching

M. PARRINELLO, Stuttgart E.W. SCHLAG, Garching W. ZINTH, Munich Hungary
P. ORMOS, Szeged

Israel
R.B. GERBER, Jerusalem
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
E. POLLAK, Rehovot

Italy
G. CICCOTTI, Rome

Janan

H. HAMAGUCHI, Tokyo M. ITO, Okazaki T. KITAGAWA, Okazaki T. KOBAYASHI, Tokyo K. YOSHIHARA, Ishikawa

The Netherlands
D. FRENKEL, Amsterdam

Russian Federation V.S. LETOKHOV, Moscow

Sweden R. RIGLER, Stockholm Switzerland H. FISCHER, Zurich S. LEUTWYLER, Bern

Taiwan Y.T. LEE, Taipei United Kingdom

A.D. BUCKINGHAM, Cambridge D.C. CLARY, London D.A. KING, Cambridge P.A. MADDEN, Oxford J.P. SIMONS, Oxford

USA
A.C. ALBRECHT, Ithaca, NY
A.C. ALBRECHT, Ithaca, NY
P. ALIVISATOS, Berkeley, CA
V.A. APKARIAN, Irvine, CA
P.F. BARBARA, Austin, TX
R. BERSOHN, New York, NY
S.G. BOXER, Stanford, CA
S.T. CEYER, Cambridge, MA
K.A. DILL, San Francisco, CA
W.A. EATON, Bethesda, MD
M.D. FAYER, Stanford, CA
G.R. FLEMING, Berkeley, CA
G. FLYNN, New York, NY
R.A. FRIESNER, New York, NY
M. KLEIN, Philadelphia, PA

USA (continued)
W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
D.M. NEUMARK, Berkeley, CA
M.D. NEWTON, Upton, NY
C.S. PARMENTER, Bloomington, IN
M.A. RATNER, Evanston, IL
G.W. ROBINSON, Lubbock, TX
G.J. SMALL, Ames, IA
J.C. TULLY, New Haven, CT
J.D. WEEKS, College Park, MD
K.B. WHALEY, Berkeley, CA
P.G. WOLYNES, Urbana, IL

R.N. ZARE, Stanford, CA

A.H. ZEWAIL, Pasadena, CA

Abstracted/indexed in: Chemical abstracts, ERDA Abstracts, ISI Currents Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physical Briefs.

Chemical Physics

Editors

ROBIN M. HOCHSTRASSER, Philadelphia
G. LUDWIG HOFACKER, Munich
H. PETER TROMMSDORFF, Grenoble

n,IN

D

tracts.

Associate Editor

DAVID CHANDLER, Berkeley

MASTER INDEX

VOLUMES 251-260

JANUARY-OCTOBER 2000



Amsterdam - Lausanne - New York - Oxford - Shannon - Tokyo

This journal and the individual contributions contained in it are protected under copyright by Elsevier Science B.V., and the following terms and conditions apply to their use:

Photocopying

Single photocopies of single articles may be made for personal use as allowed by national copyright laws. Permission of the Publisher and payment of a fee is required for all other photocopying, including multiple or systematic copying, copying for advertising or promotional purposes, resale, and all forms of document delivery. Special rates are available for educational institutions that wish to make photocopies for non-profit educational classroom use.

Permissions may be sought directly from Elsevier Science Global Rights Department, P.O. Box 800, Oxford OX5 1DX, UK; phone: (+44) 1865 843830, fax: (+44) 1865 853333, e-mail: permissions@elsevier.co.uk. You may also contact Global Rights directly through Elsevier's home page (http://www.elsevier.nl), selecting 'Obtaining Permissions'.

In the USA, users may clear permissions and make payments through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA; phone: (+1) (978) 7508400, fax: (+1) (978) 7504744, and in the UK through the Copyright Licensing Agency Rapid Clearance Service (CLARCS), 90 Tottenham Court Road, London W1P0LP, UK; phone: (+44) 20 7631 5555; fax: (+44) 20 7631 5500. Other countries may have a local reprographic rights agency for payments.

Derivative Works

Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions.

Permission of the Publisher is required for resale or distribution outside the institution.

Permission of the Publisher is required for all other derivative works, including compilations and translations.

Electronic Storage or Usage

Permission of the Publisher is required to store or use electronically any material contained in this journal, including any article or part of an article.

Except as outlined above, no part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without prior written permission of the Publisher.

Address permissions requests to: Elsevier Science Global Rights Department, at the mail, fax and e-mail addresses noted above.

Notice

No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Because of rapid advances in the medical sciences, in particular, independent verification of diagnoses and drug dosages should be made.

Although all advertising material is expected to conform to ethical (medical) standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Elsevier Science B.V Tel: (+31-20)4852-800 Fax: (+31-20)4852-775 E-mail: e.hovens@elsevier.nl

Postal Address

Chemical Physics Elsevier Science B.V. P.O. Box 2759 1000 CT Amsterdam The Netherlands

Courier Service Address

Chemical Physics Elsevier Science B.V. Sara Burgerhartstraat 25 1055 KV Amsterdam The Netherlands

The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper)

Printed in the Netherlands.

Contents

g

er or to

e: gh

ng nx:

eir

art by

ity, ein. be

Author index to volumes 251-260	1	microwave	48
		infrared	48
Subject index to volumes 251-260	33	Raman	49
		UV	50
METHODS AND CONSTRUCTS	33	visible	50
		Photon counting and phase fluorimetry	51
Theoretical	33	Photoelectron and Auger spectroscopy	51
Computational methods for electronic structure	33	Multiphoton ionization	52
CI and valence bond approach	35	X-ray spectroscopy	52
perturbative and many body approaches	36	Electron impact spectroscopy	52
density functional theory	36	Laser induced fluorescence	53
Semiempirical methods	38	Ultrafast measurements	54
Algebraic approaches	38	Nonlinear optics and spectroscopy	55
Relativistic electronic structure theory	38	Synchrotron spectroscopies	56
Wavefunctions for highly excited and unbound states	39	Coherent optical spectroscopy Optical pumping	56
Spin states and magnetic interactions	39	Multiple resonance spectroscopy	57 57
Molecular response to external fields (incl. optical	27	Optoacoustic spectroscopy	57
susceptibilities, dichroism, hyperpolarizabilities)	39	Atomic and molecular beam techniques	57
Radiative (incl. relativistic) effects on molecules and	27	Mass spectroscopy	57
molecular processes	40	Radiolysis	58
Scattering of waves and particles	41	X-ray, electron and neutron diffraction	58
Collisional and reactive molecular dynamics with non-		Neutron scattering (inelastic and quasielastic)	58
frictional forces	41	Small angle X-ray and neutron diffraction	58
Reactive molecular dynamics including dissipative pro-		Light scattering	58
cesses	41	Scanning tunneling and force microscopies	58
Intramolecular dynamics	42	Calorimetric methods	59
Molecular dynamics of many particle systems and		Measurement of macroscopic variables	59
condensed phases	43		
Quasiparticle dynamics (incl. excitons, polarons)	44	OBJECTS	59
Migration and interaction on grids and lattices	44		
Statistical computational methods (incl. Monte Carlo)	44	D !!	50
Dynamics of structures, lattices and macromolecular		Bulk systems Gases	59
conformations	45	Supersonic beams	59
Fluctuations and random processes	45	Liquids neat	61
Non-equilibrium statistical mechanics	45	Liquid mixtures and solutions	61
Non-equilibrium thermodynamic and hydrodynamic theories	46	Crystals	64
Equilibrium statistical mechanics and thermodynamics	46	neat	64
Extremum methods for ensembles (energy, entropy, free	40	mixed	64
energy)	46	Glasses	65
Time and space correlation functions	46	Complex fluids	65
		liquid crystals	65
		micelles	65
Experiment	47	Polymers	65
Magnetic resonances	47	Semiconductors	66
Molecular spectroscopy	47	Metals and alloys	66

Contents

intensities	87
nd nuclear motion	88
3	88
processes	89
	90
	91
S	91
distribution (incl. vibrational	
	92
elds and lifetimes	92
	92
l. optical)	93
	93
ion)	93
	94
	94
	95
	95
	95
om transfer	96
m transier	96
g states)	97
diffusive)	97
diffusive)	97
	98
ccitations	98
Keitations	98
	98
	98
	99
	99
	99
	99
	99
ses	
nsport properties	99
ds and glasses	100
phase transitions	100
and -organization	101
function relationships	101
	and -organization function relationships

Author index to volumes 251-260

Abduranman, A., A. Shukla and M. Dolg, Correlated ground-state ab initio	
calculations of polymethineimine	257 (2000) 301
Abematsu, C., see Nakayama, H.	253 (2000) 331
Abram, U., see Voigt, A.	253 (2000) 171
Adachi, H., see Suzuki, C.	253 (2000) 27
Adamovich, I.V., see Plönjes, E.	256 (2000) 315
Adamovich, I.V., see Plönjes, E.	260 (2000) 353
Adamowicz, L., see Al-Jihad, I.	257 (2000) 167
Adamowicz, L., see Smith, D.M.A.	260 (2000) 45
Adhikari, S. and G.D. Billing, The geometric phase effect in chemical reactions	259 (2000) 149
Agostini, G., L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and	
A. Hirsch, Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash	
photolysis and time-resolved EPR study	253 (2000) 105
Agranovich, V.M., see Hoffmann, M.	258 (2000) 73
Ägren, H., see Plashkevych, O.	260 (2000) 11
Alemán, C., The keto-amino/enol tautomerism of cytosine in aqueous solution. A	
theoretical study using combined discrete/self-consistent reaction field models	253 (2000) 13
Alikhani, E.M., see Krim, L.	254 (2000) 267
Alikhani, M.E., see Asselin, P.	256 (2000) 195
Al-Jihad, I., J. Smets and L. Adamowicz, Isomerism of the covalent anion of the dimer	
of uracil and 1-methyl-cytosine: ab initio study	257 (2000) 167
Allouche, A.R., see Korek, M.	256 (2000) 1
Aloisio, S. and J.S. Francisco, A density functional study of H ₂ O–OClO, (H ₂ O) ₂ –OClO	
and H ₂ O-ClOO complexes	254 (2000) 1
Al-Quraishi, A.A., see Moore, B.G.	252 (2000) 337
Alvarez, C., see Correia, N.T.	252 (2000) 151
Andersson, P.U., see Marković, N.	252 (2000) 409
Andersson, S., N. Marković and G. Nyman, Quasi-classical trajectory simulations of	
C + NO crossed molecular beam experiments	259 (2000) 99
Andrews, L., see Galland, N.	255 (2000) 205
Andrews, L., see Kushto, G.P.	257 (2000) 223
Angulo, G., see Galán, M.	254 (2000) 329
Aramendía, P.F., see Torga, J.R.	253 (2000) 249

Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z	
Asselin, P., P. Soulard, M.E. Alikhani and J.P. Perchard, Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and	
supersonic jet-FTIR experiments	256 (2000) 195
Aubert-Frécon, M., see Korek, M.	256 (2000) 1
Azria, R., see Tronc, M.	254 (2000) 69
Babinec, P., see Roszak, S.	256 (2000) 177
Badenes, M.P., E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri, Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂	253 (2000) 205
Bae, S.Y., IJ. Lee and J. Park, Methylation effects on the collisional quenching of	255 (2000) 102
vibrationally excited benzene derivatives by unexcited parent molecules	255 (2000) 103
Bae, Y.C., see Kim, I.H.	260 (2000) 337
Baer, M., Topological effects in molecular systems: an attempt towards a complete	252 (2000) 122
theory	259 (2000) 123
Baer, T., see Kim, D.	256 (2000) 251
Bagryansky, V.A., O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N. Molin, Quantum beats in recombination of spin-correlated radical ion pairs with equivalent	
protons	255 (2000) 237
Bailey, W.C., DFT and HF-DFT calculations of ¹⁴ N quadmpole coupling constants in	
molecules	252 (2000) 57
Bailey, W.C., F.M. Gonzalez and J. Castiglione, Density functional theory and Hartree–Fock-density functional theory calculations of ¹⁷ O, ³³ S, and ⁷³ Ge	
quadrupole coupling constants	260 (2000) 327
Bakker, H.J., S. Woutersen and HK. Nienhuys, Reorientational motion and	
hydrogen-bond stretching dynamics in liquid water	258 (2000) 233
Bakker, H.J., see van den Broek, M.A.F.H.	253 (2000) 157
Balta, B. and F.A. Gianturco, Structural properties and quantum effects in protonated	
helium clusters. I. The ab initio interaction potential	254 (2000) 203
Balta, B., F.A. Gianturco and F. Paesani, Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller	
aggregates	254 (2000) 215
Bandyopadhyay, P., P.K. Bharadwaj, M. Basu Roy, R. Dutta and S. Ghosh, Photophysical properties of tris-acetylpyrene derivative of a cryptand in different	
environments	255 (2000) 325
Baraille, I., see Dupin, H.	256 (2000) 7
Baranović, G., see Stepanić, V.	254 (2000) 151
Barnes, A.C., see Ramos, S.	258 (2000) 171
Bartolotti, L.J., see Chesnut, D.B.	253 (2000) 1
Bartolotti, L.J., see Chesnut, D.B.	257 (2000) 175
Barvík, I., Ch. Warns, Th. Neidlinger and P. Reineker, Erratum to: "Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units:	
influence of quasi-static and dynamic disorder" [Chem. Phys. 240 (2000) 173-189]	255 (2000) 403
Basiev, T.T., see Fedorov, V.V.	257 (2000) 275
Basilevsky, M.V., see Vener, M.V.	254 (2000) 249
Basu Roy, M., see Bandyopadhyay, P.	255 (2000) 325
Baumgärtel, H., see Hoxha, A.	256 (2000) 239
Baumgärtel, H., see Hoxha, A.	260 (2000) 237
Baumgärtel, H., see Locht, R.	257 (2000) 283

	9
Baumgärtel, H., see Schwell, M.	260 (2000) 261
Baumgarten, M., see Karabunarliev, S.	254 (2000) 239
Beck, W., see Fedorov, V.V.	257 (2000) 275
Belchior, J.C., see Braga, J.P.	260 (2000) 347
Belinsky, M.I., Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of	
ferredoxins with high-spin $S = 3/2$ ground state	255 (2000) 23
Belinsky, M.I., see Palii, A.V.	255 (2000) 51
Bellissent-Funel, MC., see Dellerue, S.	258 (2000) 315
Benderskii, V.A. and E.V. Vetoshkin, Tunneling splittings in vibrational spectra of non-	
rigid molecules	257 (2000) 203
Bennington, S.M., see Dawidowski, J.	258 (2000) 247
Ben-Nun, M. and T.J. Martínez, Photodynamics of ethylene: ab initio studies of conical	
intersections	259 (2000) 237
Berberan-Santos, M.N., J.P.S. Farinha and J.M.G. Martinho, Linear and convolution	
methods for the analysis of ground and excited state kinetics. Application to the	
monomer-excimer scheme	260 (2000) 401
Berberan-Santos, M.N., see Bodunov, E.N.	259 (2000) 49
Bergman, D.L., Topological properties of the hydrogen-bond network in liquid	()
water	253 (2000) 267
Bermejo, F.J., see Dawidowski, J.	258 (2000) 247
Bersohn, R., see Ogi, Y.	255 (2000) 379
Berthold, W., U. Höfer, P. Feulner and D. Menzel, Influence of Xe adlayer morphology	
and electronic structure on image-potential state lifetimes of Ru(0001)	251 (2000) 123
Beyer, T., B.M. Nestmann and S.D. Peyerimhoff, Study of electron polarization and	
correlation effects in resonant and background electron scattering off CF ₃ Cl	255 (2000) 1
Bharadwaj, P.K., see Bandyopadhyay, P.	255 (2000) 325
Bhattacharyya, S.P., see Chaudhury, P.	253 (2000) 295
Bibinov, N.K., A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov, Optical	200 (2000) 200
transitions from the chlorine $0^+_{11}(^3P_2)$ ion-pair state	254 (2000) 89
Bich, E., see Bock, S.	257 (2000) 147
Bielschowsky, C.E., see Rocha, A.B.	253 (2000) 51
Bigot, JY., V. Halté, JC. Merle and A. Daunois, Electron dynamics in metallic	200 (2000) 01
nanoparticles	251 (2000) 181
Billard, I., see Bockstahl, F.	256 (2000) 307
Billing, G.D., see Adhikari, S.	259 (2000) 149
Biskupič, S., see Lukeš, V.	257 (2000) 157
Bittererová, M., see Lukeš, V.	257 (2000) 157
Blaise, P. and O. Henri-Rousseau, Spectral density of medium strength H-bonds. Direct	201 (2000) 101
damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic	
approximation	256 (2000) 85
Bleyer, A., see Lane, P.A.	257 (2000) 41
BliB, B., U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy, Supersonic jet and	201 (2000) 11
solution studies of intramolecular complexes with TICT formation mimicking	
solute-solvent interaction	254 (2000) 407
Blokhin, A.P. and M.F. Gelin, Effect of collisions on the orientational relaxation of	231 (2000) 401
photofragments	252 (2000) 323
Blokhin, A.P., see Gelin, M.F.	255 (2000) 111
Blomberg, C., see Edholm, O.	252 (2000) 221
0, -1, 000 200000000000000000000000000000000	202 (2000) 221

Bock, S., E. Bich and E. Vogel, A new intermolecular potential energy surface for	255 (2000) 145
carbon dioxide from ab initio calculations	257 (2000) 147
Bockstahl, F., E. Pachoud, G. Duplâtre and I. Billard, Size of sodium dodecyl sulphate	
micelles in aqueous NaCl solutions as studied by positron annihilation lifetime	256 (2000) 207
spectroscopy	256 (2000) 307
Bodunov, E.N., M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G. Martinho,	
Eigenvalue spectrum of the survival probability of excitation in nonradiative energy	250 (2000) 40
transport Boendgen, G., see Saalfrank, P.	259 (2000) 49 251 (2000) 51
Boggs, J.E., see Demaison, J.	260 (2000) 65
Bohr, H., see Frimand, K.	255 (2000) 165
Bonamy, J., see Bruet, X.	254 (2000) 297
Bordat, P., M. Orrit, R. Brown and A. Würger, The anomalous Stark effect of single	234 (2000) 297
terrylene molecules in <i>p</i> -terphenyl crystals	258 (2000) 63
Bornemann, C. and M. Klessinger, Conical intersections and photoreactions of 2H-	230 (2000) 03
azirines	259 (2000) 263
Borovkov, V.I., see Bagryansky, V.A.	255 (2000) 237
Borras-Almenar, J.J., J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S.	255 (2000) 257
Tsukerblat, Anisotropic double exchange in orbitally degenerate mixed valence	
systems	254 (2000) 275
Böttcher, R., see Voigt, A.	253 (2000) 171
Boulet, P., F. Gilardoni, J. Weber, H. Chermette and Y. Ellinger, Reply to Comment	200 (2000) 111
on "Theoretical study of interstellar hydroxylamine chemistry: protonation and	
proton transfer mediated by H ₃ ⁺ " [Chem. Phys. 253 (2000) 389–390]	253 (2000) 391
Boullant, E., see Chevreau, H.	254 (2000) 99
Bradley, D.D.C., see Lane, P.A.	257 (2000) 41
Braga, A.P., see Braga, J.P.	260 (2000) 347
Braga, J.P., M.B. de Almeida, A.P. Braga and J.C. Belchior, Hopfield neural network	
model for calculating the potential energy function from second virial data	260 (2000) 347
Brion, C.E., see Feng, R.	252 (2000) 359
Brion, C.E., see Feng, R.	255 (2000) 353
Brion, C.E., see Feng, R.	260 (2000) 29
Brion, C.E., see Feng, R.	260 (2000) 391
Brion, C.E., see Litvinyuk, I.V.	253 (2000) 41
Brown, D., A recursive Kohn variational algorithm for the Green's operator:	
application to the T-matrix	259 (2000) 11
Brown, R., see Bordat, P.	258 (2000) 63
Bruet, X., J. Bonamy and M.L. Dubernet-Tuckey, Broadening and shifting coefficients	
of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure H_2 : coupled states and	
semiclassical calculations. Comparison with experiments	254 (2000) 297
Bruno, D., see Longo, S.	256 (2000) 265
Brutschy, B., see Bliß, B.	254 (2000) 407
Buehler, E.J., E.E. Gooch, J.L. Dial and S.K. Knudson, Semiclassical energies of low-	
lying states of one-electron diatomics	253 (2000) 219
Bussac, M.N., see Miomandre, F.	255 (2000) 291
Cabaleiro-Lago, E.M. and M.A. Ríos, Ab initio study of M(CH ₃ CN) _n clusters	A#4 (A000)
$(M = Li^+, Na^+, Mg^{2+})$ in the gas phase	254 (2000) 11

Author maex to volumes 251-260	2
Cabaleiro-Lago, E.M., see García-Muruais, A.	254 (2000) 109
Cabrillo, C., see Dawidowski, J.	258 (2000) 247
Cacace, F. and G. de Petris, Comment on "Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by H ₃ ⁺ " [Chem.	
Phys. 244 (2000) 163–174]	253 (2000) 389
Cacelli, I., R. Moccia and A. Rizzo, Gaussian type orbitals basis sets for the calculation of continuum properties in molecules: the differential photoionization cross section	252 (2000) (7
of acetylene	252 (2000) 67
Cai, MQ., L. Zhang, BY. Tang, MD. Chen, GW. Yang and KL. Han,	255 (2000) 202
Quasiclassical calculation of the chemical reaction Sr + HF Cai, MQ., L. Zhang, BY. Tang, MD. Chen, GW. Yang and KL. Han, Erratum	255 (2000) 283
to "Quasiclassical calculation of the chemical reaction Sr + HF" [Chem. Phys. 255	
(2000) 283–289]	260 (2000) 281
Callan, J.P., A.MT. Kim, L. Huang and E. Mazur, Ultrafast electron and lattice	
dynamics in semiconductors at high excited carrier densities	251 (2000) 167
Camou, J.M., see Lacombe, S.	258 (2000) 1
Cao, X. and G. Fischer, Infrared spectra of monomeric L-alanine and L-alanine-N-d ₃	
zwitterions isolated in a KBr matrix	255 (2000) 195
Capitan, M.J., see Ramos, S.	258 (2000) 171
Capitelli, M., see Esposito, F.	257 (2000) 193
Caputo, M.C., see Zitto, M.E.	259 (2000) 1
Carey, C., YK. Cheng and P.J. Rossky, Hydration structure of the α-chymotrypsin	
substrate binding pocket: the impact of constrained geometry	258 (2000) 415
Carravetta, V., see Plashkevych, O.	260 (2000) 11
Carvajal, M., R. Lemus, A. Frank, C. Jung and E. Ziemniak, An extended SU(2) model	
for coupled Morse oscillators	260 (2000) 105
Cascales, C., G. Lozano, C. Zaldo and P. Porcher, Optical spectroscopy and crystal-	
field effects on the paramagnetic susceptibility of rare-earth germanates GaRGe ₂ O ₇ ,	
R = Pr, Nd	257 (2000) 29
Cassidei, L., see Petrella, G.	256 (2000) 259
Castaño, F., see Longarte, A.	260 (2000) 83
Castaño, F., see Merelas, I.	254 (2000) 77
Castellano, E., see Badenes, M.P.	253 (2000) 205
Castiglione, J., see Bailey, W.C.	260 (2000) 327
Cataliotti, R.S., P. Sassi, A. Morresi and G. Paliani, Mandelstam-Brillouin spectra and hyperacoustic velocities dispersion of trideuteroacetonitrile in the liquid	()
state	255 (2000) 85
Cataliotti, R.S., see Morresi, A.	254 (2000) 337
Cavell, R.G., see Jürgensen, A.	257 (2000) 123
Cederbaum, L.S., see Mahapatra, S.	259 (2000) 211
Chaalan, A., see Korek, M.	256 (2000) 1
Chae, WS., see Kang, SG.	256 (2000) 295
Chambaud, G., see Robbe, J.M.	
Chandra, A.K., M.T. Nguyen and T. Zeegers-Huyskens, Density functional calcula-	252 (2000) 9
tions on simple carbonyl bases: protonation and hydrogen bond formation with	
water	255 (2000) 149
Chang, YM., L. Xu and H.W.K. Tom, Coherent phonon spectroscopy of GaAs	
surfaces using time-resolved second-harmonic generation	251 (2000) 283

Chatzis, G. and J. Samios, The isotopic and temperature dependent properties of	
hydrogen chloride dissolved in carbon tetrachloride. A molecular dynamics	
approach	257 (2000) 51
Chaudhury, P., S.P. Bhattacharyya and W. Quapp, A genetic algorithm based	
technique for locating first-order saddle point using a gradient dominated recipe	253 (2000) 295
Chauhan, A.S., R. Ravi and R.P. Chhabra, Self-diffusion in liquid metals	252 (2000) 227
Chemla, D.S., see Wegener, M.	251 (2000) 269
Chen, F.Z., D.L. Judge and C.Y.R. Wu, Temperature dependent photoabsorption	
cross sections of allene and methylacetylene in the VUV-UV region	260 (2000) 215
Chen, M., see Zhang, L.	254 (2000) 231
Chen, M., X. Wang, L. Zhang, Q. Qin and Q. Zheng, Photomobility of O(1D) atom in	
solid Ar and its reaction with CF ₃ I	255 (2000) 95
Chen, MD., see Cai, MQ.	255 (2000) 283
Chen, MD., see Cai, MQ.	260 (2000) 281
Chen, X.J., see Zhang, C.F.	256 (2000) 275
Cheng, YK., see Carey, C.	258 (2000) 415
Chermette, H., see Boulet, P.	253 (2000) 391
Chernukho, A.P., see Plönjes, E.	256 (2000) 315
Chesnut, D.B. and L.J. Bartolotti, The electron localization function description of	
aromaticity in five-membered rings	253 (2000) 1
Chesnut, D.B. and L.J. Bartolotti, The pair density description of aromaticity in some	
substituted cyclopentadienyl systems: a comparison of AIM and ELF bonding	
descriptors	257 (2000) 175
Chevreau, H., E. Boullant, C. Dézarnaud-Dandine and A. Sevin, A theoretical	
exploratory study of low-energy (1-2 eV) electron catalysis in the $CO_2 + H_2 \rightarrow$	
HCOOH gas phase process	254 (2000) 99
Cheyssac, P., see Stagira, S.	251 (2000) 259
Chhabra, R.P., see Chauhan, A.S.	252 (2000) 227
Chialvo, A.A., E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson, The	
structure of water from 25°C to 457°C: comparison between neutron scattering and	
molecular simulation	258 (2000) 109
Chiang, TC., Photoemission linewidths narrower than the quasiparticle inverse	
lifetime	251 (2000) 133
Chidley, M.D., see Plönjes, E.	260 (2000) 353
Chien, L.C., see Ostroverkhov, V.	257 (2000) 263
Chikhaoui, A., see Kustova, E.V.	255 (2000) 59
Cho, B.R., see Kim, S.	256 (2000) 289
Cho, SI., see Shin, S.	259 (2000) 27
Choi, JH., Spectral properties and ligand field analysis of cis-dinitrito(1,4,8,11-	
tetraazacyclotetradecane)chromium(III) nitrate	256 (2000) 29
Choi, Y.J., see Park, S.J.	257 (2000) 135
Chotin, JL., see Schwell, M.	260 (2000) 261
Chowdhury, P.K., Impulsive IR-multiphoton dissociation of acrolein: observation of	
non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR	
fluorescence spectroscopy	260 (2000) 151
Christophorov, L.N., A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik,	
Structure-function self-organization in nonequilibrium macromolecular systems	256 (2000) 45
Chu, YC., see Walrafen, G.E.	258 (2000) 427

	,
Chulkov, E.V., see Echenique, P.M.	251 (2000) 1
Ciriaco, F., see Petrella, G.	256 (2000) 259
Cisowski, J., see Mazurak, Z.	254 (2000) 25
Citra, A., see Kushto, G.P.	257 (2000) 223
Clemente-Juan, J.M., see Borras-Almenar, J.J.	254 (2000) 275
Cloutier, P., see Tronc, M.	254 (2000) 69
Coat, Y.L., see Tronc, M.	254 (2000) 69
Cobos, C.J., see Badenes, M.P.	253 (2000) 205
Combellas, C., F. Kajzar, G. Mathey, M.A. Petit and A. Thiébault, Zwitterionic	
polymers for nonlinear optics	252 (2000) 165
Cong, SL., KL. Han, GZ. He and NQ. Lou, Determination of population,	(,
orientation and alignment of symmetric top molecule using laser-induced fluores-	
cence	256 (2000) 225
Congeduti, A., M. Nardone and P. Postorino, Polarized Raman spectra of a single	
crystal of iodine	256 (2000) 117
Conrad, U., see Hohlfeld, J.	251 (2000) 237
Cooper, G., see Feng, R.	252 (2000) 359
Cooper, G., see Feng, R.	255 (2000) 353
Cooper, G., see Feng, R.	260 (2000) 29
Cooper, G., see Feng, R.	260 (2000) 391
Coronado, E., see Borras-Almenar, J.J.	254 (2000) 275
Correia, N.T., C. Alvarez, J.J. Moura Ramos and M. Descamps, Molecular motions in	
molecular glasses as studied by thermally stimulated depolarisation currents (TSDC) Costela, A., see Holzer, W.	252 (2000) 151
Croce, A.E., see Badenes, M.P.	256 (2000) 125
	253 (2000) 205
Čuma, M., U.W. Schmitt and G.A. Voth, A multi-state empirical valence bond model	250 (2000) 107
for acid-base chemistry in aqueous solution Cummings, P.T., see Chialvo, A.A.	258 (2000) 187
Czaja, M., see Mazurak, Z.	258 (2000) 109
Czaja, M., see Mazurak, Z.	254 (2000) 25
da Silveira, N.P., F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto,	
Ab initio determination of the $C_6H_6\cdots CS_2$ cluster stabilization energy	253 (2000) 165
Dagher, M., see Korek, M.	256 (2000) 1
Dai, HL., see Sjodin, T.	251 (2000) 205
Dargelos, A., see Dupin, H.	256 (2000) 7
Dargelos, A., see Lacombe, S.	258 (2000) 1
Daub, J., see Ern, J.	259 (2000) 331
Daunois, A., see Bigot, JY.	251 (2000) 181
Dawidowski, J., F.J. Bermejo, C. Cabrillo and S.M. Bennington, Generalized frequency	
spectra of water at both sides of the freezing transition	258 (2000) 247
de Almeida, M.B., see Braga, J.P.	260 (2000) 347
de Oliveira Jr., Z.T. and M.C. dos Santos, Semi-empirical study of chain conformation	
and absorption spectra of polyanilines: size, solvent and disorder effects	260 (2000) 95
de Petris, G., see Cacace, F.	253 (2000) 389
De Silvestri, S., see Stagira, S.	251 (2000) 259
Dehareng, D., see Hoxha, A.	256 (2000) 239
	moo (2000) 201
Dehareng, D., see Hoxha, A.	260 (2000) 237

Del Festi N. E. Velle, C. Fleteric V. Herrende and A. N. L	
Del Fatti, N., F. Vallée, C. Flytzanis, Y. Hamanaka and A. Nakamura, Electron	251 (2000) 215
dynamics and surface plasmon resonance nonlinearities in metal nanoparticles Dellerue, S. and MC. Bellissent-Funel, Relaxational dynamics of water molecules at	251 (2000) 215
protein surface	259 (2000) 215
Demaison, J., L. Margulès and J.E. Boggs, The equilibrium N-H bond length	258 (2000) 315
Derecskei-Kovacs, A., see Li, R.	260 (2000) 65
	254 (2000) 309
Descamps, M., see Correia, N.T.	252 (2000) 151
Dézarnaud-Dandine, C., see Chevreau, H.ü	254 (2000) 99
Dial, J.L., see Buehler, E.J. Dietz, F., see Tyutyulkov, N.	253 (2000) 219
	255 (2000) 223
Dimitrova, Y. and S. Peyerimhoff, Ab initio study of structures of hydrogen-bonded nitric acid complexes	254 (2000) 125
Ding, F., see Kushto, G.P.	254 (2000) 125
	257 (2000) 223
Ding, S., see Guan, D.	252 (2000) 179
Ding, S., see Zheng, Y.	255 (2000) 217
Došlić, N. and O. Kühn, Monitoring laser driven hydrogen atom motion by transient	255 (2000) 247
infrared spectroscopy	255 (2000) 247
Doetschman, D.C., D.C. Gilbert and D.W. Dwyer, Li cation–aromatic organic radical	256 (2000) 25
complex in a zeolite studied by electron spin echo envelope modulation spectroscopy	256 (2000) 37
Dohnálek, Z., see Smith, R.S.	258 (2000) 291
Doktorov, A.B., see Toropov, Yu.V.	253 (2000) 231
Dolg, M., see Abdurahman, A.	257 (2000) 301
Domcke, W., see Kühl, A.	259 (2000) 227
Domcke, W., see Sobolewski, A.L.	259 (2000) 181
Dore, J., Structural studies of water in confined geometry by neutron diffraction	258 (2000) 327
dos Santos, M.C., see de Oliveira, Z.T.	260 (2000) 95
Driesner, T., see Chialvo, A.A.	258 (2000) 109
Duan, YB., see Mukhopadhyay, I.	257 (2000) 91
Duarte, F.J., see Holzer, W.	256 (2000) 125
Dubernet-Tuckey, M.L., see Bruet, X.	254 (2000) 297
Dulieu, F.v., see Schwell, M.	260 (2000) 261
Dupin, H., I. Baraille, C. Larrieu and A. Dargelos, Theoretical study of the infrared	
and ultraviolet spectrum of the radical F ₂ CN	256 (2000) 7
Duplâtre, G., see Bockstahl, F.	256 (2000) 307
Duran, M., see Forés, M.	260 (2000) 53
Dutta, R., see Bandyopadhyay, P.	255 (2000) 325
Dwyer, D.W., see Doetschman, D.C.	256 (2000) 37
Echenique, P.M., J.M. Pitarke, E.V. Chulkov and A. Rubio, Theory of inelastic	
lifetimes of low-energy electrons in metals	251 (2000) 1
Edholm, O. and C. Blomberg, Stretched exponentials and barrier distributions	251 (2000) 1
Edvardsson, D., see Holland, D.M.P.	252 (2000) 221
Edvardsson, D., see Holland, D.M.P.	252 (2000) 257
Edvardsson, D., see Potts, A.W.	253 (2000) 133
El Gridani, A. and M. El Mouhtadi, Electronic and structural properties of CaH ₂ : an	254 (2000) 385
ab initio Hartree–Fock study	252 (2000)
	252 (2000) 1
Fl Mouhtadi M. see El Gridani A	, ,
El Mouhtadi, M., see El Gridani, A. Eland, J.H.D., see Wilsey, S.	252 (2000) 1 258 (2000) 21

Ellinger, Y., see Boulet, P.	253 (2000)	391
Elstner, M., K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai,		
DFT studies on helix formation in N-acetyl-(L-alanyl) _n -N'-methylamide for $n = 1-20$	256 (2000)	15
Ern, J., M. Petermann, T. Mrozek, J. Daub, K. Kuldová and C. Kryschi,		
Dihydroazulene/vinylheptafulvene photochromism: dynamics of the photochemical		
ring-opening reaction	259 (2000)	331
Esposito, F., M. Capitelli and C. Gorse, Quasi-classical dynamics and vibrational		
kinetics of $N^+N_2(v)$ system	257 (2000)	193
Eustatiu, I.G., J.T. Francis, T. Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P.		
Hitchcock, Generalized oscillator strengths for inner-shell excitation of SF ₆ re-		
corded with a high-performance electron energy loss spectrometer	257 (2000)	235
Evans, C.M., J.D. Scott, F.H. Watson and G.L. Findley, Photoionization studies of		
C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆	260 (2000)	225
Fakherddin, K., see Korek, M.	256 (2000)	1
Farantos, S.C., see Froudakis, G.E.	258 (2000)	13
Farinha, J.P.S., see Berberan-Santos, M.N.	260 (2000)	401
Fateev, A.A., see Bibinov, N.K.	254 (2000)	89
Faure, A., L. Wiesenfeld and P. Valiron, Temperature dependence of fast neutral-		
neutral reactions: a triatomic model study	254 (2000)	49
Fauster, T., C. Reuß, I.L. Shumay and M. Weinelt, Femtosecond two-photon		
photoemission studies of image-potential states	251 (2000)	111
Fedorov, A.V. and D.L. Snavely, Direct correlation method for OH, NH and CH local		
modes: vibrational overtone spectroscopy of biphenyl, anthracene, isobutanol,		
2-chloroethanol and ethylenediamine at the third overtone region	254 (2000)	169
Fedorov, V.V., W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis, Fine level		
splitting of aggregate neodymium centers in CaF ₂ crystals	257 (2000)	
Feller, KH., see Malyshev, V.A.	254 (2000)	31
Feng, R., G. Cooper and C.E. Brion, Quantitative studies of the photoabsorption of		
carbonyl sulphide in the valence-shell, S 2p, 2s and C Is inner-shell regions (4-360		
eV) by dipole electron impact spectroscopies	252 (2000)	359
Feng, R., G. Cooper and C.E. Brion, UV, VUV and soft X-ray photoabsorption of		
dimethyl ether by dipole (e,e) spectroscopies	260 (2000)	391
Feng, R., G. Cooper, Y. Sakai and C.E. Brion, Dipole (e,e+ion) coincidence studies of		
the ionic photofragmentation and photoionization of carbonyl sulfide in the valence	255 (2000)	252
shell and S 2p, 2s and C 1s inner shell regions (10–300 eV)	255 (2000)	353
Feng, R., Y. Sakai, Y. Zheng, G. Cooper and C.E. Brion, Orbital imaging for the		
valence shell of sulphur dioxide: comparison of EMS measurements with near	260 (2000)	20
Hartree–Fock limit and density functional theory	260 (2000)	
Fernández, J.A., see Merelas, I. Fernández, J.A., see Longarte, A.	254 (2000)	
Ferrari, L., A proper mobility formula for large, heavy particles in gases in any regime	260 (2000) 257 (2000)	
Ferraro, M.B., see Zitto, M.E.	257 (2000)	
Ferretti, A., A. Lami and G. Villani, A model study of the wavepacket dynamics	239 (2000)	1
around a Jahn–Teller conical intersection in a symmetric charge-transfer system	259 (2000)	201
Feulner, P., see Berthold, W.	251 (2000)	
Findley, G.L., see Evans, C.M.	260 (2000)	
Finger, K., see Saalfrank, P.	251 (2000)	
	(====)	-

Fischer, G. and P. Wormell, Vibronic analyses of the lowest singlet-singlet and singlet-	
triplet band systems of pyridazine	257 (2000) 1
Fischer, G., see Cao, X.	255 (2000) 195
Flytzanis, C., see Del Fatti, N.	251 (2000) 215
Flytzanis, C., see Fedorov, V.V.	257 (2000) 275
Forés, M., M. Duran and M. Solà, Substituent effects on the intramolecular proton	201 (2000) 210
transfer in the ground and lowest-lying singlet excited states of salicylaldimine	260 (2000) 53
Fouassier, J.P., see Ley, C.	255 (2000) 335
Fourkas, J.T., see Loughnane, B.J.	253 (2000) 323
Francis, J.T., see Eustatiu, I.G.	257 (2000) 235
Francisco, J.S., see Aloisio, S.	
Franco, M.L., see Jorge, F.E.	
	253 (2000) 21
Frank, A., see Carvajal, M.	260 (2000) 105
Frauenheim, Th., see Elstner, M.	256 (2000) 15
Frimand, K., H. Bohr, K.J. Jalkanen and S. Suhai, Structures, vibrational absorption and vibrational circular dichroism spectra of L-alanine in aqueous solution: a density	
functional theory and RHF study	255 (2000) 165
Fritz, T., see Hoffmann, M.	258 (2000) 73
Fritzsche, S., R. Haberlandt and M. Wolfsberg, Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual	
interaction in the diffusion of methane in a cation-free LTA zeolite	253 (2000) 283
Froudakis, G.E., S.C. Farantos and M. Velegrakis, Mass spectra and theoretical	()
modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters	258 (2000) 13
Fuß, W., see Trushin, S.A.	259 (2000) 313
Fuß, W., Y. Haas and S. Zilberg, Twin states and conical intersections in linear polyenes	259 (2000) 273
Fujimoto, H., see Kimura, T.	253 (2000) 125
Fukuhara, M., A.H. Matsui and M. Takeshima, Low-temperature elastic anomalies in	255 (2000) 125
an anthracene single crystal	258 (2000) 97
Fuster, F. and B. Silvi, Determination of protonation sites in bases from topological rules	252 (2000) 279
ruster, r. and B. Shvi, Determination of protonation sites in bases from topological rules	232 (2000) 219
Gadzuk, J.W., Hot-electron femtochemistry at surfaces: on the role of multiple electron	
processes in desorption	251 (2000) 87
Gaffney, K.J., C.M. Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris,	251 (2000) 07
Femtosecond electron dynamics at the benzene/Ag(111) interface	251 (2000) 99
Gagliardi, L., N.C. Handy, CK. Skylaris and A. Willetts, A theoretical study of	231 (2000) 77
plutonium diketone complexes for solvent extraction	252 (2000) 47
Galán, M. and G. Angulo, Some remarks on the application of relaxation techniques to	232 (2000) 47
chemical equilibria	254 (2000) 220
Galasso, V., D. Jones, A. Modelli and M.L. Trudell, A study of the molecular structure	254 (2000) 329
and spectroscopic properties of benzo- and pyrido-tetraazapentalenes	254 (2000) 375
Galiazzo, G., see Marri, E.	260 (2000) 383
Galland, N., Y. Hannachi, D.V. Lanzisera and L. Andrews, Theoretical study of	
structures, energetics and vibrational properties of BC ₂ H ₅ species	255 (2000) 205
García, A.E., see Hummer, G.	258 (2000) 349
García-Moreno, I., see Holzer, W.	256 (2000) 125
García-Muruais, A., E.M. Cabaleiro-Lago, J.M. Hermida-Ramón and M.A. Ríos, The study of $A(CH_3OH)_{1-6}$ ($A = Li^+$, Na^+) in the gas phase based on ab initio	
calculations, analysis of the solvation process	254 (2000) 109

	**
Garde, S., see Hummer, G.	258 (2000) 349
Gauduel, Y. and H. Gelabert, Primary steps of an electron-proton reaction in aqueous	
electrolyte solutions	256 (2000) 333
Gée, C., see Schwell, M.	260 (2000) 261
Gelabert, H., see Gauduel, Y.	256 (2000) 333
Gelin, M.F., see Blokhin, A.P.	252 (2000) 323
Gelin, M.F., V.A. Tolkachev and A.P. Blokhin, Semiclassical description of purely rotational recurrences for collisionless asymmetric top molecules: new results	255 (2000) 111
Gerhards, M., see Roth, W.	252 (2000) 247
Ghosh, S., see Bandyopadhyay, P.	255 (2000) 325
Ghosh, S.K., see Samanta, A.	254 (2000) 39
Gianturco, F.A., see Balta, B.	254 (2000) 203
Gianturco, F.A., see Balta, B.	254 (2000) 215
Gilardoni, F., see Boulet, P.	253 (2000) 391
Gilbert, D.C., see Doetschman, D.C.	256 (2000) 37
Glaeske, H., see Malyshev, V.A.	254 (2000) 31
Glasbeek, M., see Humbs, W.	254 (2000) 319
Glebov, E.M., V.F. Plyusnin, N.V. Tkachenko and H. Lemmetyinen, Laser flash	20 , (2000) 217
photolysis of IrCl ₆ ²⁻ in aqueous solutions	257 (2000) 79
Goez, M. and V. Zubarev, Light intensity dependence of a two-photon catalytic cycle:	237 (2000) 12
photoionization via absorption–electron transfer–absorption	256 (2000) 107
Gole, J.L., see McQuaid, M.J.	260 (2000) 367
Gómez, J.A. and D. Guenzburger, Density functional study of electronic, magnetic and	200 (2000) 507
hyperfine properties of $[M(CN)_5NO]^{2-}$ (M = Fe, Ru) and reduction products	253 (2000) 73
Gonzalez, F.M., see Bailey, W.C.	260 (2000) 327
Gooch, E.E., see Buehler, E.J.	253 (2000) 219
Gooding, E., see Kholodenko, Y.	259 (2000) 71
Gorse, C., see Esposito, F.	257 (2000) 193
Gosnell, T.R., see Lobad, A.I.	251 (2000) 227
Goworek, T., T. Suzuki, E. Hamada, K. Kondo and Y. Ito, Pressure quenching of positronium in solid biphenyl	
Granucci, G., see Santoro, F.	255 (2000) 347
	259 (2000) 193
Gratz, H. and A. Penzkofer, Singlet-singlet excited-state absorption and triplet-triplet	0.5.4 (0.000) 0.5
absorption of <i>meso</i> -tetraphenylporphine	254 (2000) 363
Gratz, H., see Holzer, W.	256 (2000) 125
Gu, Y., see Hou, H.	252 (2000) 17
Guan, D., see Zheng, Y. Guan, D., X. Yi, Y. Zheng, S. Ding and J. Sun, Dynamical Lie algebraic approach to	255 (2000) 273
rotationally inelastic scattering of molecules from surfaces	252 (2000) 179
Güdde, J., see Hohlfeld, J.	251 (2000) 237
Gudiksen, M.S., see Sander, M.U.	258 (2000) 25
Guenzburger, D., see Gómez, J.A.	253 (2000) 73
Guo, SL., see Zhu, XL.	253 (2000) 24
Haas, Y., see Fuß, W.	250 (2000) 27
Haas, Y., see Zilberg, S.	259 (2000) 273
Haberlandt, R., see Fritzsche, S.	259 (2000) 249
Haberiandi, A., see Fillzsche, S.	253 (2000) 283

Hagler, T.W., see Lane, P.A.	257 (2000) 41
Hahn, S. and G. Stock, Femtosecond secondary emission arising from the nonadiabatic	
photoisomerization in rhodopsin	259 (2000) 297
Halkier, A., B. Kirchner, H. Huber and M. Jaszuński, Nuclear quadrupole coupling	
constant of 21 Ne in the neon dimer and its influence on the T_1 NMR relaxation time	252 (2000) 102
in fluid neon	253 (2000) 183
Hallbrucker, A., see Pichler, A.	258 (2000) 391
Halté, V., see Bigot, JY.	251 (2000) 181
Hamada, E., see Goworek, T.	255 (2000) 347
Hamanaka, Y., see Del Fatti, N.	251 (2000) 215
Han, JG., WM. Pang and YY. Shi, Theoretical study on the sandwich clusters of	257 (2000) 21
Na _n (COT) _m by density functional method	257 (2000) 21
Han, KL., see Cai, MQ.	255 (2000) 283
Han, KL., see Cai, MQ.	260 (2000) 281
Han, KL., see Cong. SL.	256 (2000) 225
Handy, N.C., see Gagliardi, L.	252 (2000) 47
Hannachi, Y., see Galland, N.	255 (2000) 205
Hansen, M.J., A.A. Neufeld and J.B. Pedersen, Recombination yield of geminate	
radical pairs in high magnetic fields: general results and application to free	260 (2000) 125
diffusion	260 (2000) 125
Harano, Y., H. Sato and F. Hirata, A theoretical study on a Diels-Alder reaction	
in ambient and supercritical water: viewing solvent effects through frontier orbitals	259 (2000) 151
	258 (2000) 151
Harris, C.B., see Gaffney, K.J.	251 (2000) 99
Harris, F.M., see Jeffreys, N.	260 (2000) 295
Harris, K.D.M., see Turner, G.W.	256 (2000) 159
Hasche, T., see Hoffmann, M. Hashimoto, Y., see Kimura, T.	258 (2000) 73
	253 (2000) 125
Haver M.A. con Potts, A.W.	260 (2000) 415
Hayes, M.A., see Potts, A.W. He, FC., see Li, XY.	254 (2000) 385
He, GZ., see Cong, SL.	260 (2000) 283
Heimann, J., see Mazurak, Z.	256 (2000) 225
Helmi, M.S., see Roston, G.D.	254 (2000) 25 258 (2000) 55
Hemmerling, B., see Hubschmid, W.	259 (2000) 109
Henri-Rousseau, O., see Blaise, P.	256 (2000) 85
Hermida-Ramón, J.M., see García-Muruais, A.	254 (2000) 109
Hidalgo, A., see Tolosa, S.	255 (2000) 73
Hirata, F., see Harano, Y.	258 (2000) 151
Hiraya, A., see Kanda, K.	255 (2000) 369
Hirsch, A., see Agostini, G.	253 (2000) 105
Hitchcock, A.P., see Eustatiu, I.G.	257 (2000) 235
Hlady, J.C. and R.P. Steer, Electronic spectroscopy and structures of the van der Waals	237 (2000) 233
complexes of α , ω -dihaloalkanes with anthracene	260 (2000) 249
Hoatson, G.L., see Kristensen, J.H.	252 (2000) 97
Hochstrasser, R.M., see Kholodenko, Y.	259 (2000) 71
Höfer, U., see Berthold, W.	251 (2000) 123

Hoffmann, M., K. Schmidt, T. Fritz, T. Hasche, V.M. Agranovich and K. Leo, The lowest energy Frenkel and charge-transfer excitons in quasi-one-dimensional		
structures: application to MePTCDI and PTCDA crystals Hohlfeld, J., SS. Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias,	258 (2000)	73
Electron and lattice dynamics following optical excitation of metals	251 (2000)	237
Holland, D.M.P., D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen, An experimental and theoretical study of the valence shell		
photoelectron spectrum of bromobenzene Holland, D.M.P., D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von. Niessen, A systematic investigation of the influence of Cooper minima	252 (2000)	
on the photoionisation dynamics of the monohalobenzenes	253 (2000)	
Holland, D.M.P., see Potts, A.W.	254 (2000)	385
Holzer, W., H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte, Photo-physical characterization of rhodamine 6G in a 2-		
hydroxyethyl-methacrylate methyl-methacrylate copolymer	256 (2000)	125
Holzwarth, A.R., see Christophorov, L.N.	256 (2000)	45
Homeier, H.H.H., see Strasser, J.	255 (2000)	301
Hottmann, K., see Hoxha, A.	256 (2000)	239
Hottmann, K., see Hoxha, A.	260 (2000)	237
Hou, H., B. Wang and Y. Gu, The attractive quartet potential energy surface for the		
$CH_3C(a^4A_2) + CO$ reaction	252 (2000)	17
Hovorun, D.M., see Shishkin, O.V.	260 (2000)	317
Hoxha, A., R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H. Baumgärtel, Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the		
ionic B state	256 (2000)	239
Hoxha, A., R. Locht, B. Leyh, D. Dehareng, K. Hottmann, H.W. Jochims and H. Baumgärtel, The photoabsorption and constant ionic state spectroscopy of		
vinylbromide	260 (2000)	
Hoxha, A., see Locht, R.	257 (2000)	
Hu, X.K., see Mao, D.M.	257 (2000)	253
Huang, L., see Callan, J.P.	251 (2000)	167
Hubač, I., see Urban, J.	255 (2000)	
Huber, H., see Halkier, A.	253 (2000)	183
Hubschmid, W. and B. Hemmerling, Relaxation processes in singlet O ₂ analyzed by		
laser-induced gratings Humbs, W., H. Zhang and M. Glasbeek, Femtosecond fluorescence upconversion	259 (2000)	109
spectroscopy of vapor-deposited tris(8-hydroxyquinoline) aluminum films Hummer, G., S. Garde, A.E. García and L.R. Pratt, New perspectives on hydrophobic	254 (2000)	319
effects	259 (2000)	240
Hupp, J.T., see Vance, F.W.	258 (2000)	
Husain, D., see Merelas, I.	253 (2000)	
Hwang, DY. and A.M. Mebel, Ab initio study of spin-forbidden unimolecular	254 (2000)	11
decomposition of carbon dioxide	256 (2000)	169
Hwang, DY. and A.M. Mebel, Ab initio study of the reaction mechanism of singlet		
and triplet N ₂ O and their intersystem crossing	259 (2000)	89
Hwang, J., see Kim, S.	256 (2000)	289
Hynes, J.T., see Morita, A.	258 (2000)	371

14	A	Author index to volumes 251–200		
F	Iynes, J.T., see Peslherbe, G.H.		258 (2000)	201
I		and T. Kushida, Determination of single-site disordered materials by double site-selective		
	spectroscopy		259 (2000)	63
I	m Kang, T., see Kim, S.		256 (2000)	289
	mhof, P., see Roth, W.		252 (2000)	247
I	and nonlinear static electric properti	d A.J. Sadlej, Vibrational corrections to linear ies of polyatomic molecules at non-optimum	260 (2000)	1
T	reference geometry		260 (2000)	
	nishi, H., see Okamoto, H.		260 (2000) 252 (2000)	
	shchenko, V.N., see Makarov, V.I. shii, K., see Nakayama, H.		253 (2000)	
		carrier gas effect under nucleation in thermal	255 (2000)	331
1	diffusion chambers	carrier gas effect under frueleation in thermal	256 (2000)	61
T	to, Y., see Goworek, T.		255 (2000)	
	zvekov, V., see Kovács, A.		253 (2000)	
1	zvekov, v., see Rovaes, A.		255 (2000)	173
1	acques, P., see Ley, C.		255 (2000)	335
	ähnke, V., see Hohlfeld, J.		251 (2000)	
	albout, A.F., see Smith, D.M.A.		260 (2000)	
	alkanen, K.J., see Elstner, M.		256 (2000)	
	alkanen, K.J., see Frimand, K.		255 (2000)	
	anssen, R.A.J., see Meskers, S.C.J.		260 (2000)	
	aszuński, M., see Halkier, A.		253 (2000)	
		s, Vertical triple ionization of ethyne molecules with O^{2+} beam ions	260 (2000)	
1	leung, GH., see Park, S.J.	itii O bealli iolis	257 (2000)	
	Jochims, H.W., see Hoxha, A.		260 (2000)	
	Jochims, H.W., see Locht, R.		257 (2000)	
	Jochims, HW., see Schwell, M.		260 (2000)	
		at capacity feature of annealed ices and ice	258 (2000)	
1	Johari, G.P., see McAnanama, J.G.	intusivity in terms of the entropy	252 (2000)	
	Johnston, R.L., see Turner, G.W.		256 (2000)	
	Jones, D., see Galasso, V.		254 (2000)	
		sal Gaussian basis set for positive and negative	25 . (2000)	5,0
	ions from H through Xe	and and and are too positive and negative	253 (2000)	21
	Judge, D.L., see Chen, F.Z.		260 (2000)	
	Jung, C., see Carvajal, M.		260 (2000)	
	Jung, JS., see Kang, SG.		256 (2000)	
	Jung, KH., see Lee, SH.		260 (2000)	
	Jung, YJ., see Lee, SH.		260 (2000)	
	relaxation paths in 9,9'-bianthryl ar	, Y.H. Meyer and W. Rettig, Excited state and 9-carbazolyl-anthracene: a sub-ps transient		
	absorption study		253 (2000)	339
	Jurczok, M., P. Plaza, W. Rettig and acceptor substituted bianthryl deriva	M.M. Martin, Ultrafast electron transfer in tives	256 (2000)	137

	15
Jürgensen, A. and R.G. Cavell, A comparison of the oxygen 1s photoabsorption spectra	
of SO_2 and NO_2	257 (2000) 123
Jurlewicz, A., see Kozłowski, M.	252 (2000) 289
Kajzar, F., see Combellas, C.	252 (2000) 165
Kanda, K., M. Kono, T. Nagata, A. Hiraya, K. Tabayashi and K. Shobatake,	
Photodissociation spectroscopy of ClCN in the vacuum ultraviolet region	255 (2000) 369
Kanematsu, Y., see Ichino, Y.	259 (2000) 63
Kang, SG., WS. Chae, YR. Kim, JS. Jung and SH. Lee, Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the distance estimation	
between trap sites	256 (2000) 295
Kang, T.I., see Kim, S.	256 (2000) 289
Karabunarliev, S. and M. Baumgarten, Using antiferromagnetic couplers for high-spin	
ground states in ion radicals	254 (2000) 239
Karasik, A.Ya., see Fedorov, V.V.	257 (2000) 275
Karlsson, L., see Holland, D.M.P.	252 (2000) 257
Karlsson, L., see Holland, D.M.P.	253 (2000) 133
Karlsson, L., see Potts, A.W.	254 (2000) 385
Kawai, J., see Suzuki, C.	253 (2000) 27
Kay, B.D., see Smith, R.S.	258 (2000) 291
Keresztury, G., see Kovács, A.	253 (2000) 193
Kharkyanen, V.N., see Christophorov, L.N.	256 (2000) 45
Khmelinskii, I.V., see Makarov, V.I.	252 (2000) 379
Kholodenko, Y., M. Volk, E. Gooding and R.M. Hochstrasser, Energy dissipation and	
relaxation processes in deoxy myoglobin after photoexcitation in the Soret region	259 (2000) 71
Kilcoyne, A.L.D., see Eustatiu, I.G.	257 (2000) 235
Kim, D. and T. Baer, Gas-phase measurement of ΔH^0 between axial and equatorial	
conformations of 3-methylcyclopentanone	256 (2000) 251
Kim, HS., Monte Carlo simulation study of solvent effect on Na ⁺ to Li ⁺ ion mutation	253 (2000) 305
Kim, HS., Solvent effect on Sr ²⁺ to Ca ²⁺ ion mutation: Monte Carlo simulation study Kim, I.H. and Y.C. Bae, A modified perturbed hard-sphere-chain equation of state:	257 (2000) 183
consideration of attractive contribution	260 (2000) 337
Kim, S., H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T.I. Kang and B.R. Cho, First	200 (2000) 337
hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward	
monolithic molecular materials for photorefractivity	256 (2000) 289
Kim, YR., see Kang, SG.	256 (2000) 295
Kimmel, G.A., see Smith, R.S.	258 (2000) 291
Kimura, T., M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki, Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission	230 (2000) 27
spectroscopy	253 (2000) 125
Kirchner, B., see Halkier, A.	253 (2000) 183
Kirmse, R., see Voigt, A.	253 (2000) 173
Kim, A.MT., see Callan, J.P.	251 (2000) 16
Klein, M.L., see Yarne, D.A.	258 (2000) 163
Kleinermanns, K., see Roth, W.	252 (2000) 241
Klessinger, M., see Bornemann, C.	259 (2000) 263
Klokishner, S., J. Linares and F. Varret, Effect of hydrostatic pressure on phase	
transitions in spin-crossover 1D systems	255 (2000) 317

V Malanana la Maran Flatana M	256 (2000) 15
Knapp-Mohammady, M., see Elstner, M.	256 (2000) 15
Knowles, P.J., see Robbe, J.M. Knudson, S.K., see Buehler, E.J.	252 (2000) 9
	253 (2000) 219
Kobeissi, M., see Korek, M.	256 (2000) 1
Kobzeva, T.V., see Bagryansky, V.A.	255 (2000) 237
Kochubei, S.A., see Makarov, V.I.	252 (2000) 379
Kofman, R., see Stagira, S.	251 (2000) 259
Kohler, HH., see Treml, H.	252 (2000) 199
Kohtani, S., see Okamoto, H.	260 (2000) 193
Kok, A., P.A.Z. van Emmichoven and A. Niehaus, State selected reactions of krypton	2.50 (2000) 45
ions with methane	258 (2000) 47
Kokh, D.B., see Bibinov, N.K.	254 (2000) 89
Kołodziej, H.A., see Kozłowski, M.	252 (2000) 289
Kondo, K., see Goworek, T.	255 (2000) 347
Kono, M., see Kanda, K.	255 (2000) 369
Köppel, H., see Mahapatra, S.	259 (2000) 211
Korek, M., A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M. Aubert-Frécon, Theoretical study of the electronic structure of the LiRb and	
NaRb molecules	256 (2000) 1
Korolkov, M.V. and KM. Weitzel, The predissociation dynamics of vibrational eigenstates in the $A^2\Sigma^+$ state of HBr ⁺ ions: numerical solution of coupled time-dependent	
Schrödinger equations	252 (2000) 209
Kosuge, M., see Moriyama, M.	253 (2000) 91
Kovács, A., G. Keresztury and V. Izvekov, Intramolecular hydrogen-bonding in	
2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study	253 (2000) 193
Kovačević, B., see Maksić, Z.B.	253 (2000) 59
Kozlov, G.G., see Malyshev, V.A.	254 (2000) 31
Kozłowski, M., H.A. Kołodziej, R. Wieczorek, Z. Latajka and A. Jurlewicz, Dielectric relaxation and molecular conformational energy of some arylazo benzothiazine	
derivatives	252 (2000) 289
Krim, L., C. Prot, E.M. Alikhani and L. Manceron, Reactions of ground state Ti atoms	
with NO: insertion versus complexation. An IR matrix isolation study	254 (2000) 267
Kristensen, J.H., G.L. Hoatson and R.L. Vold, Motional effects on optimum coherence	
transfer in ² H MAS NMR spectroscopy	252 (2000) 97
Kryschi, C., see Ern, J.	259 (2000) 331
Kühl, A. and W. Domcke, Effect of a dissipative environment on the dynamics at a	
conical intersection	259 (2000) 227
Kühn, O., see Došlić, N.	255 (2000) 247
Kuldová, K., see Ern, J.	259 (2000) 331
Küpper, J., see Schmitt, M.	254 (2000) 349
Kurita, A., see Ichino, Y.	259 (2000) 63
Kurosaki, Y., see Umemoto, H.	259 (2000) 39
Kusalik, P.G., see Svishchev, I.M.	258 (2000) 181
Kushida, T., see Ichino, Y.	259 (2000) 63
Kushto, G.P., F. Ding, B. Liang, X. Wang, A. Citra and L. Andrews, Infrared spectra	(====)
of BeNO and MgNO in solid argon	257 (2000) 223
Kustova, E.V. and A. Chikhaoui, Kinetic modelling of radiative reacting gas flow under	
strong nonequilibrium conditions	255 (2000) 59

Author maex to volumes 251-200	17
Kuznetsov, D.S., V.B. Morozov, A.N. Olenin and V.G. Tunkin, High resolution study of	
1388 cm ⁻¹ CO ₂ vibration by time-domain CARS: spectral exchange and Dicke effect	257 (2000) 117
Kwon, C, see Lobad, A.I.	251 (2000) 227
LaBerge, L.J. and J.C. Tully, A rigorous procedure for combining molecular dynamics	
and Monte Carlo simulation algorithms	260 (2000) 183
Lacabanne, C., see Samouillan, V.	255 (2000) 259
Lacombe, S., M. Loudet, A. Dargelos and J.M. Camou, Calculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of	250 (2000)
configuration interaction methods	258 (2000) 1
Ladanyi, B.M., see Peslherbe, G.H.	258 (2000) 201
Lami, A., see Ferretti, A.	259 (2000) 201
Lamparth, I., see Agostini, G.	253 (2000) 105
Lamure, A., see Samouillan, V.	255 (2000) 259
Lane, P.A., H. Mellor, S.J. Martin, T.W. Hagler, A. Bleyer and D.D.C. Bradley,	
Electroabsorption spectroscopy of distyrylbenzene derivatives	257 (2000) 41
Lanzisera, D.V., see Galland, N.	255 (2000) 205
Larrieu, C., see Dupin, H.	256 (2000) 7
Latajka, Z., see Kozłowski, M.	252 (2000) 289
Laurinc, V., see Lukeš, V.	257 (2000) 157
Lazzeretti, P., see Zitto, M.E.	259 (2000) 1
Leach, S., see Schwell, M.	260 (2000) 261
LeCoat, Y., See Tronc, M.	254 (2000) 69
Lee, IJ., see Bae, S.Y.	255 (2000) 103
Lee, SH., see Kang, SG.	256 (2000) 295
Lee, SH., YJ. Jung and KH. Jung, Photodissociation dynamics of CH ₂ BrCl at 234 nm	260 (2000) 143
Lee, W., see Plönjes, E.	,
Lee, Y.S., see Park, S.J.	260 (2000) 353
Legay, F. and N. Legay-Sommaire, High resolution near infrared spectrum of solid	257 (2000) 135
nitrogen, pure and doped with carbon dioxide	257 (2000) 102
Legay-Sommaire, N., see Legay, F.	257 (2000) 103
	257 (2000) 103
Lemmetyinen, H., see Glebov, E.M.	257 (2000) 79
Lempert, W.R., see Plönjes, E.	260 (2000) 353
Lemus, R., see Carvajal, M.	260 (2000) 105
Leo, K., see Hoffmann, M.	258 (2000) 73
Lesar, A., see Maksić, Z.B.	253 (2000) 59
Leszczynski, J., see Roszak, S.	256 (2000) 177
Leszczynski, J., see Shishkin, O.V.	260 (2000) 317
Ley, C., F. Morlet-Savary, P. Jacques and J.P. Fouassier, Solvent dependence of the intersystem crossing kinetics of thioxanthone	255 (2000) 335
Leyh, B., see Hoxha, A.	256 (2000) 239
Leyh, B., see Hoxha, A.	260 (2000) 237
Leyh, B., see Locht, R.	257 (2000) 283
Li, CM., see Sjodin, T.	251 (2000) 205
Li, R., A. Derecskei-Kovacs and S.W. North, The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler	20. (2000) 200
spectroscopy	254 (2000) 309
*	, , ,

Li, XY., J. Tong and FC. He, Ab initio calculation for inner reorganization energy of	
gas-phase electron transfer in organic molecule-ion systems	260 (2000) 283
Liang, B., see Kushto, G.P.	257 (2000) 223
Liedl, K.R., see Pichler, A.	258 (2000) 391
Linares, J., see Klokishner, S.	255 (2000) 317
Lipson, R.H., see Mao, D.M.	257 (2000) 253
Litvinyuk, I.V., Y. Zheng and C.E. Brion, Valence shell orbital imaging in adamantane	237 (2000) 233
by electron momentum spectroscopy	253 (2000) 41
Liu, S.H., see Gaffney, K.J.	251 (2000) 99
Livotto, P.R., see da Silveira, N.P.	253 (2000) 165
Lobad, A.I., A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell, Laser induced	255 (2000) 105
	251 (2000) 227
dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MuO ₃	251 (2000) 227
Locht, R., B. Leyh, A. Hoxha, D. Dehareng, H.W. Jochims and H. Baumgärtel, About	
the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine	257 (2000) 202
structure and its vibrational analysis	257 (2000) 283
Locht, R., see Hoxha, A.	256 (2000) 239
Locht, R., see Hoxha, A.	260 (2000) 237
Lommatzsch, U., see Bliß, B.	254 (2000) 407
Longarte, A., J.A. Fernández, I. Unamuno and F. Castaño, Structure and ground and	
first electronic excited state vibrational modes of the ethyl-p-aminobenzoate	2(0 (2000) 82
conformers	260 (2000) 83
Longo, S., D. Bruno and P. Minelli, Direct simulation of non-linear interparticle	256 (2000) 265
collisional relaxation of ensembles of two-level systems	256 (2000) 265
Lou, NQ., see Cong, SL.	256 (2000) 225
Loudet, M., see Lacombe, S.	258 (2000) 1
Loughnane, B.J., A. Scodinu and J.T. Fourkas, Temperature-dependent optical Kerr	
effect spectroscopy of chloroform in restricted geometries	253 (2000) 323
Lozano, G., see Cascales, C.	257 (2000) 29
Lugovoj, E.V., see Bibinov, N.K.	254 (2000) 89
Lukeš, V., M. Bittererová, V. Laurinc and S. Biskupič, Ab initio study of the $F_2(X^1\Sigma_g^+)$	
H(² S) van der Waals complex	257 (2000) 157
Luther, K., see Sander, M.U.	258 (2000) 257
Luzar, A., Extent of inter-hydrogen bond correlations in water. Temperature effect	258 (2000) 267
Lynch, G.C. and B.M. Pettitt, Semi-grand canonical molecular dynamics simulation of	
bovine pancreatic trypsin inhibitor	258 (2000) 405
Ma, D., see Zheng, N.W.	258 (2000) 37
MacDonald, M.A., see Potts, A.W.	254 (2000) 385
Mach, P., see Urban, J.	255 (2000) 15
Madurga, S., J.C. Paniagua and E. Vilaseca, Solvent effect on conformational	
equilibrium: a Monte Carlo study of 1,3-dichloropropane in carbon tetrachloride	255 (2000) 123
Maggini, M., see Agostini, G.	253 (2000) 105
Mahapatra, S., H. Köppel, L.S. Cederbaum, P. Stampfuß and W. Wenzel,	
Nonadiabatic wave packet dynamics on the coupled X^2A_1/A^2B_2 electronic states	
of NO ₂ based on new ab initio potential energy surfaces	259 (2000) 211
Makarov, V.I. and E. Quiñones, Relaxation of individual rotational levels of the	
$\tilde{A}^1 A_u$ electronic state of acetylene excited to the $2v_3'$ and $(v_1' + v_3' + v_6')$ vibrational	
modes	253 (2000) 259

11 09 55

.65 .25

Author maex to blumes 251-200	19
Makarov, V.I., I.V. Khmelinskii, S.A. Kochubei and V.N. Ishchenko, Magnetic	
fluorescence quenching of the NO $\beta(0-9)$ transition	252 (2000) 379
Maksić, Z.B., B. Kovačević and A. Lesar, Protonation of archetypal aromatic and	
antiaromatic systems - G2 studies of benzene and cyclobutadiene	253 (2000) 59
Malyshev, V.A., G.G. Kozlov, H. Glaeske and KH. Feller, Channels of the exciton-	
exciton annihilation in one-dimensional aggregates at low temperature	254 (2000) 31
Manceron, L., see Krim, L.	254 (2000) 267
Mandal, A.K. and M.K. Pal, Strong fluorescence emissions by H-aggregates of the dye	
thiacyanine in the presence of the surfactant aerosol-OT	253 (2000) 115
Mao, D.M., X.K. Hu, Y.J. Shi and R.H. Lipson, Dispersive photoelectron spectro-	
scopy of the ungerade Rydberg states of Xe ₂ near Xe*(6p,5d)	257 (2000) 253
Marconi, M.C., see Torga, J.R.	253 (2000) 249
Margulès, L., see Demaison, J.	260 (2000) 65
Maripuu, R., see Holland, D.M.P.	252 (2000) 257
Maripuu, R., see Holland, D.M.P.	253 (2000) 133
Maripuu, R., see Potts, A.W.	254 (2000) 385
Marković, N., P.U. Andersson, M.B. Någråd and J.B.C. Pettersson, Erratum to	
"Scattering of water from graphite: simulations and experiments". [Chem. Phys. 247	
(2000) 413–430]	252 (2000) 409
Marković, N., see Andersson, S.	259 (2000) 99
Marri, E., G. Galiazzo, U. Mazzucato and A. Spalletti, Effect of solvent polarizability	
on dual fluorescence of EE-1-phenyl,4-(1'-pyrenyl)-1,3-butadiene	260 (2000) 383
Martín Negri, R., see Torga, J.R.	253 (2000) 249
Martínez, T.J., see Ben-Nun, M.	259 (2000) 237
Martin, M.M., see Jurczok, M.	253 (2000) 339
Martin, M.M., see Jurczok, M.	256 (2000) 137
Martin, S.J., see Lane, P.A.	257 (2000) 41
Martinho, J.M.G., see Berberan-Santos, M.N.	260 (2000) 401
Martinho, J.M.G., see Bodunov, E.N.	259 (2000) 49
Mášik, J., see Urban, J.	255 (2000) 15
Mathey, G., see Combellas, C.	252 (2000) 165
Matsui, A.H., see Fukuhara, M.	258 (2000) 97
Matsuzaki, S., see Kimura, T.	253 (2000) 125
Matthias, E., see Hohlfeld, J.	251 (2000) 237
Matzdorf, R., Quasi-particle lifetimes on noble metal surfaces studied by ARPES and	
STM	251 (2000) 151
Mayer, E., see Pichler, A.	258 (2000) 391
Mazur, E., see Callan, J.P.	251 (2000) 167
Mazurak, Z., J. Cisowski, J. Heimann, A. Nateprov and M. Czaja, Magnetic	
susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium	254 (2000) 25
Mazzucato, U., see Marri, E.	260 (2000) 383
McAnanama, J.G., D.A. Wasylyshyn and G.P. Johari, Temperature-independent onset of diffusion control during polymerization in a diepoxide-amine mixture by	
dielectric measurements	252 (2000) 237
McNeill, J.D., see Gaffney, K.J.	251 (2000) 99
McQuaid, M.J. and J.L. Gole, The effect of carbonyl complexation on highly	()
exothermic vanadium oxidation reactions	260 (2000) 367
Mebel, A.M., see Hwang, DY.	256 (2000) 169

Mebel, A.M., see Hwang, DY.	259 (2000) 89
Mellor, H., see Lane, P.A.	257 (2000) 41
Meng, Q., see Zheng, Y.	255 (2000) 273
Menzel, D., see Berthold, W.	251 (2000) 123
Menzel, D., see Wurth, W.	251 (2000) 141
Merelas, I., J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño, The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and	
$CCl_2(A^1B_1(0,7,0))$ by rare gases and simple molecules	254 (2000) 77
Merle, JC., see Bigot, JY.	251 (2000) 181
Meskers, S.C.J., R.A.J. Janssen, J.E.M. Haverkort and J.H. Wolter, Relaxation of	
photo-excitations in films of oligo- and poly-(para-phenylene vinylene) derivatives	260 (2000) 415
Meyer, Y.H., see Jurczok, M.	253 (2000) 339
Mihailović, D., see Umek, P.	253 (2000) 361
Miller, A.D., see Gaffney, K.J.	251 (2000) 99
Minaev, B.F., Oxygen absorption below and near the Herzberg I continuum. Ab initio	
calculation of the transitions probability from metastable states	252 (2000) 25
Minagawa, Y., see Nakayama, H.	253 (2000) 331
Minelli, P., see Longo, S.	256 (2000) 265
Miomandre, F., M.N. Bussac, E. Vieil and L. Zuppiroli, Influence of the local electric	
field on ionic transport during redox switching of conducting polymers	255 (2000) 291
Moccia, R., see Cacelli, I.	252 (2000) 67
Modelli, A., see Galasso, V.	254 (2000) 375
Molin, Yu.N., see Bagryansky, V.A.	255 (2000) 237
Molin, Yu.N., see Toropov, Yu.V.	253 (2000) 231
Molinari, E. and M. Tomellini, Non-equilibrium vibrational kinetics in adlayers:	
outline of an alternative approach to catalytic processes	253 (2000) 367
Monnerville, M., see Robbe, J.M.	252 (2000) 9
Monte, C., see Bliß, B.	254 (2000) 407
Monti, S., see Agostini, G.	253 (2000) 105
Moon, H., see Kim, S.	256 (2000) 289
Moore, B.G. and A.A. Al-Quraishi, The structure of liquid clusters of Lennard-Jones	
atoms	252 (2000) 337
Morita, A. and J.T. Hynes, A theoretical analysis of the sum frequency generation	
spectrum of the water surface	258 (2000) 371
Moriyama, M., M. Kosuge, S. Tobita and H. Shizuka, Excited-state intramolecular proton transfer followed by <i>cis-trans</i> isomerization of (1-hydroxy-2-naphthyl)-s-	, ,
triazine derivatives	253 (2000) 91
Morlet-Savary, F., see Ley, C.	255 (2000) 335
Morozov, V.B., see Kuznetsov, D.S.	257 (2000) 117
Morresi, A., P. Sassi, M. Paolantoni, S. Santini and R.S. Cataliotti, Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid	201 (200)
acetonitrile and acetonitrile-d ₃	254 (2000) 337
Morresi, A., see Cataliotti, R.S.	255 (2000) 85
Moura Ramos, J.J., see Correia, N.T.	252 (2000) 151
Mrozek, T., see Ern, J.	259 (2000) 331
Mukhopadhyay, I. and YB. Duan, Analysis of torsion-rotational transitions in the	
first three torsional states of CH ₃ OD	257 (2000) 91
Mukoyama, T., see Suzuki, C.	253 (2000) 27

	21
Müllen, K., see Tyutyulkov, N.	255 (2000) 223
Nagano, H., see Petek, H.	251 (2000) 71
Nagata, T., see Kanda, K.	255 (2000) 369
Någråd, M.B., see Marković, N.	252 (2000) 409
Naguleswaran, S., M.F. Reid and G.E. Stedman, Prediction of pure electric-dipole two-	(-;)
photon absorption circular dichroism in lanthanide compounds	256 (2000) 207
Nakagaki, R., see Okamoto, H.	260 (2000) 193
Nakamura, A., see Del Fatti, N.	251 (2000) 21:
Nakamura, Y., see Okamoto, H.	260 (2000) 193
Nakano, M. and K. Yamaguchi, Electron-photon field dynamics: numerically exact calculations of multi-state molecule systems interacting with a single-mode coherent	
photon field	252 (2000) 11:
Nakayama, H., Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii, Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman	
spectra of 4-alkyl-4'-cyanobiphenyl	253 (2000) 33
Nardone, M., see Congeduti, A.	256 (2000) 11
Nateprov, A., see Mazurak, Z.	254 (2000) 2
Naumkin, F.Y., Transition intensities in rare gas triatomic ions: DIM versus point-	
charge approximation	252 (2000) 30
Neidlinger, Th., see Barvík, I.	255 (2000) 40
Neilson, G.W., see Ramos, S.	258 (2000) 17
Nestmann, B.M., see Beyer, T.	255 (2000)
Neufeld, A.A., see Hansen, M.J.	260 (2000) 12
Nguyen, M.T., see Chandra, A.K.	255 (2000) 14
Niehaus, A., see Kok, A.	258 (2000) 4
Nienhuys, HK., see Bakker, H.J.	258 (2000) 23
Niessen, W.v., see Holland, D.M.P.	253 (2000) 13
Nisoli, M., see Stagira, S.	251 (2000) 25
North, S.W., see Li, R.	254 (2000) 30
Nunes Pereira, E.J., see Bodunov, E.N.	259 (2000) 4
Nyman, G., see Andersson, S.	259 (2000) 9
Ogawa, S., see Petek, H.	251 (2000) 7
Ogi, Y., M. Takahashi, K. Tsukiyama and R. Bersohn, Laser-induced amplified	
spontaneous emission from the 3d and nf Rydberg states of NO	255 (2000) 37
Okamoto, H., H. Inishi, Y. Nakamura, S. Kohtani and R. Nakagaki, Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the ground	
state and vibrational analysis	260 (2000) 19
Olenin, A.N., see Kuznetsov, D.S.	257 (2000) 11
Omerzu, A., see Umek, P.	253 (2000) 36
Orrit, M., see Bordat, P.	258 (2000) 6
Ostroverkhov, V., O. Ostroverkhova, R.G. Petschek, K.D. Singer, L. Sukhomlinova, R.J. Twieg, SX. Wang and L.C. Chien, Optimization of the molecular	
hyperpolarizability for second harmonic generation in chiral media	257 (2000) 26
Ostroverkhova, O., see Ostroverkhov, V.	257 (2000) 26
Pachoud, E., see Bockstahl, F.	256 (2000) 30

der der	and made to commed and and	
Paesani, F., see Balta, B.		254 (2000) 215
Painelli, A., Erratum to: "Amplification o	f NLO responses: vibronic and solvent effects	
in push-pull polyenes" [Chem. Phys. 2	245 (2000) 185–197]	253 (2000) 393
Pal, M.K., see Mandal, A.K.		253 (2000) 115
Paliani, G., see Cataliotti, R.S.		255 (2000) 85
Palii, A.V., M.I. Belinsky and B.S. Tsuker	rblat, Vibronic model of hyperfine interaction	
in dimeric mixed-valence clusters		255 (2000) 51
Palii, A.V., see Borras-Almenar, J.J.		254 (2000) 275
Palm, P., see Plönjes, E.		256 (2000) 315
Palm, P., see Plönjes, E.		260 (2000) 353
Pang, WM., see Han, JG.		257 (2000) 21
Paniagua, J.C., see Madurga, S.		255 (2000) 123
Paolantoni, M., see Morresi, A.		254 (2000) 337
Papadopoulos, M.G., see Ingamells, V.E.		260 (2000) 1
Park, J., see Bae, S.Y.		255 (2000) 103
Park, S.J., Y.J. Choi, Y.S. Lee and GH.	Jeung, Ab initio calculations of the electronic	
states of KRb		257 (2000) 135
Park, S.Y., see Kim, S.		256 (2000) 289
Parry, D.E., see Jeffreys, N.		260 (2000) 295
Pasimeni, L., see Agostini, G.		253 (2000) 105
Pecina, O. and W. Schmickler, The solver	nt influence on the electrochemical transfer of	
divalent ions		252 (2000) 349
Pecul, M. and J. Sadlej, The nuclear sp	oin-spin coupling constants in methanol and	
methylamine: geometry and solvent ef	fects	255 (2000) 137
Pedersen, J.B., see Hansen, M.J.		260 (2000) 125
Pelmenschikov, A., see Shishkin, O.V.		260 (2000) 317
Penzkofer, A., see Gratz, H.		254 (2000) 363
Penzkofer, A., see Holzer, W.		256 (2000) 125
Perakis, I.E., see Shahbazyan, T.V.		251 (2000) 37
Perchard, J.P., see Asselin, P.		256 (2000) 195
Pereira, F.V., see da Silveira, N.P.		253 (2000) 165
Persico, M., see Santoro, F.		259 (2000) 193
Pesce, L., see Saalfrank, P.		251 (2000) 51
Peslherbe, G.H., B.M. Ladanyi and J.T	. Hynes, Structure of NaI ion pairs in water	
clusters		258 (2000) 201
	l S. Ogawa, The role of Auger decay in hot	
electron excitation in copper		251 (2000) 71
Petek, H., see Sjodin, T.		251 (2000) 205
Petermann, M., see Ern, J.		259 (2000) 331
Petit, M.A., see Combellas, C.		252 (2000) 165
	Order and disorder signatures in the specular	
scattering intensity of He particles from	m adsorbate covered Pt surfaces	256 (2000) 259
Petrongolo, C., see Santoro, F.		259 (2000) 193
Petsalakis, I.D. and G. Theodorakopoul	os, Electronic states of CF	254 (2000) 181
Petschek, R.G., see Ostroverkhov, V.		257 (2000) 263
Pettersson, J.B.C., see Marković, N.		252 (2000) 409
Pettitt, B.M., see Lynch, G.C.		258 (2000) 405
Peyerimhoff, S., see Dimitrova, Y.		254 (2000) 125

Author lines to columns 251-200	23
Peyerimhoff, S.D., see Beyer, T.	255 (2000) 1
Pichler, A., S. Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer, The role of water in B-DNAs B ₁ to B ₁₁ conformer substates interconversion: a combined	
study by calorimetry, FT-IR spectroscopy and computer simulation	258 (2000) 391
Pitarke, J.M., see Echenique, P.M.	251 (2000) 1
Plönjes, E., P. Palm, A.P. Chernukho, I.V. Adamovich and J.W. Rich, Time-resolved	251 (2000) 1
Fourier transform infrared spectroscopy of optically pumped carbon monoxide	256 (2000) 315
Plönjes, E., P. Palm, W. Lee, M. D. Chidley, I.V. Adamovich, W.R. Lempert and J.W. Rich, Vibrational energy storage in high pressure mixtures of diatomic	250 (2000) 515
molecules	260 (2000) 353
Plashkevych, O., T. Privalov, H. Agren, V. Carravetta and K. Ruud, On the validity of the equivalent cores approximation for computing X-ray photoemission and	
photoabsorption spectral bands	260 (2000) 11
Plaza, P., see Jurczok, M.	253 (2000) 339
Plaza, P., see Jurczok, M.	256 (2000) 137
Plyusnin, V.F., see Glebov, E.M.	257 (2000) 79
Popov, A.V., P.A. Purtov and A.V. Yurkovskaya, Calculation of CIDNP field	
dependences in biradicals in the photolysis of large-ring cycloalkanones	252 (2000) 83
Porcher, P., see Cascales, C.	257 (2000) 29
Postorino, P., see Congeduti, A.	256 (2000) 117
Potts, A.W., D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von Niessen, An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene	
molecule	254 (2000) 385
Potts, A.W., see Holland, D.M.P.	252 (2000) 257
Potts, A.W., see Holland, D.M.P.	253 (2000) 133
Prato, M., see Agostini, G.	253 (2000) 105
Pratt, L.R., see Hummer, G.	258 (2000) 349
Pravilov, A.M., see Bibinov, N.K.	254 (2000) 89
Privalov, T., see Plashkevych, O.	260 (2000) 11
Prot, C., see Krim, L.	254 (2000) 267
Purtov, P.A., see Popov, A.V.	252 (2000) 83
Puyuelo, P., see Merelas, I.	254 (2000) 77
Qin, Q., see Chen, M.	255 (2000) 95
Qin, QZ., see Zhang, L.	254 (2000) 231
Quapp, W., see Chaudhury, P.	253 (2000) 295
Quiñones, E., see Makarov, V.I.	253 (2000) 259
Rae Cho, B., see Kim, S.	256 (2000) 289
Ramos, S., A.C. Barnes, G.W. Neilson and M.J. Capitan, Anomalous X-ray diffraction	
studies of hydration effects in concentrated aqueous electrolyte solutions	258 (2000) 171
Ravi, R., see Chauhan, A.S.	252 (2000) 227
Reid, M.F., see Naguleswaran, S.	256 (2000) 207
Reineker, P., see Barvík, I.	255 (2000) 403
Reinhold, J., see Voigt, A.	253 (2000) 171
Rettig, W., see Bliß, B.	254 (2000) 407

Rettig, W., see Jurczok, M.	253 (2000) 339
Rettig, W., see Jurczok, M.	256 (2000) 137
Reuß, C., see Fauster, T.	251 (2000) 111
Rich, J.W., see Plönjes, E.	256 (2000) 315
Rich, J.W., see Plönjes, E.	260 (2000) 353
Richter, U., see Voigt, A.	253 (2000) 171
Ríos, M.A., see Cabaleiro-Lago, E.M.	254 (2000) 11
Ríos, M.A., see García-Muruais, A.	254 (2000) 109
Rizzo, A., see Cacelli, I.	252 (2000) 67
Robbe, J.M., M. Monnerville, G. Chambaud, P. Rosmus and P.J. Knowles, Theoretical	232 (2000) 07
spectroscopic data of the HO ₂ ⁺ ion	252 (2000) 9
Rocha, A.B. and C.E. Bielschowsky, Vibronic coupling for H ₂ CO and CO ₂	253 (2000) 51
Rode, B.M., see Sagarik, K.	260 (2000) 159
Rodembusch, F.S., see da Silveira, N.P.	253 (2000) 165
Rosmus, P., see Robbe, J.M.	252 (2000) 9
Rossky, P.J., see Carey, C.	258 (2000) 415
Rossky, P.J., see Soper, A.K.	258 (2000) 107
Roston, G.D. and M.S. Helmi, The interatomic potentials and dipole moments of the	236 (2000) 107
excited 1 _u state of Cd–Cd and ³ 1 state of Cd–Ar	258 (2000) 55
Rostov, I.V., see Vener, M.V.	254 (2000) 249
Roszak, S., P. Babinec and J. Leszczynski, New phenomena revealed by quantum	254 (2000) 249
chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules	256 (2000) 177
Roth, W., P. Imhof, M. Gerhards, S. Schumm and K. Kleinermanns, Reassignment of	230 (2000) 177
ground and first excited state vibrations in phenol	252 (2000) 247
Rubio, A., see Echenique, P.M.	251 (2000) 247
Rüdisser, S., see Pichler, A.	258 (2000) 391
Ruud, K., see Plashkevych, O.	260 (2000) 11
Ruzzi, M., see Agostini, G.	253 (2000) 105
Ruzzi, III., see Agostini, O.	233 (2000) 103
Saalfrank, P., G. Boendgen, K. Finger and L. Pesce, Photodesorption of NO from a	
metal surface: quantum dynamical implications of a two-mode model	251 (2000) 51
Sadlej, A.J., see Ingamells, V.E.	260 (2000) 1
Sadlej, J., see Pecul, M.	255 (2000) 137
Sagarik, K. and B.M. Rode, Intermolecular potential for benzoic acid-water based on	255 (2000) 157
the test-particle model and statistical mechanical simulations of benzoic acid in	
aqueous solutions	260 (2000) 159
Saito, N., see Suzuki, I.H.	253 (2000) 351
Sakai, Y., see Feng, R.	255 (2000) 351
Sakai, Y., see Feng, R.	260 (2000) 29
Sakaki, S., see Kimura, T.	253 (2000) 125
Samanta, A. and S.K. Ghosh, Role of inertial and non-Markovian effects on activated	255 (2000) 125
barrier crossing dynamics for charge transfer reactions in solution	254 (2000) 39
Samios, D., see da Silveira, N.P.	253 (2000) 165
Samios, J., see Chatzis, G.	257 (2000) 51
Samouillan, V., A. Lamure and C. Lacabanne, Dielectric relaxations of collagen and	237 (2000) 31
elastin in the dehydrated state	255 (2000) 250
Sanche, L., see Tronc, M.	255 (2000) 259
Desirency and the transfer transfer transfer to the transfer trans	254 (2000) 69

Author fines, to totames 237-200		23
Sánchez Rayo, M.N., see Merelas, I.	254 (2000)	77
Sander, M.U., M.S. Gudiksen, K. Luther and J. Troe, Liquid water ionization:	. (====)	
mechanistic implications of the H/D isotope effect in the geminate recombination of		
hydrated electrons	258 (2000)	257
Sansón, J.A., see Tolosa, S.	255 (2000)	73
Santini, S., see Morresi, A.	254 (2000)	337
Santoro, F., C. Petrongolo, G. Granucci and M. Persico, Quantum and semiclassical		
dynamics of the Franck-Condon wave packet on the coupled potential surfaces of		
the X^2A'/A^2A' conical intersection	259 (2000)	193
Sassi, P., see Cataliotti, R.S.	255 (2000)	85
Sassi, P., see Morresi, A.	254 (2000)	337
Sastre, R., see Holzer, W.	256 (2000)	125
Sato, H., see Harano, Y.	258 (2000)	151
Savel'ev, V.A., see Sokolov, N.D.	252 (2000)	393
Schmickler, W., see Pecina, O.	252 (2000)	349
Schmid, W.E., see Trushin, S.A.	259 (2000)	313
Schmidt, K., see Hoffmann, M.	258 (2000)	73
Schmitt, M., J. Küpper, D. Spangenberg and A. Westphal, Determination of the		
structures and barriers to hindered internal rotation of the phenol-methanol cluster		
in the S_0 and S_1 states	254 (2000)	
Schmitt, T., see Holzer, W.	256 (2000)	
Schmitt, U.W., see Cuma, M.	258 (2000)	
Schumm, S., see Roth, W.	252 (2000)	247
Schwell, M., F. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H. Baumgärtel and		
S. Leach, Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV	260 (2000)	261
photon energy range Sciortino, F., Slow dynamics in supercooled water	260 (2000)	
Scodinu, A., see Loughnane, B.J.	258 (2000)	
Scott, J.D., see Evans, C.M.	253 (2000)	
Seo, J., see Kim, S.	260 (2000)	
Sevin, A., see Chevreau, H.	256 (2000) 254 (2000)	
Shahbazyan, T.V. and LI.E. Perakis, Surface collective excitations in ultrafast pump-	254 (2000)	77
probe spectroscopy of metal nanoparticles	251 (2000)	37
Shi, Y.J., see Mao, D.M.	257 (2000)	
Shi, YY., see Han, JG.	257 (2000)	
Shin, S. and SI. Cho, Quantum dynamics of model proton-coupled electron transfer	257 (2000)	21
reactions	259 (2000)	27
Shishkin, O.V., A. Pelmenschikov, D.M. Hovorun and J. Leszczynski, Theoretical	200 (2000)	
analysis of low-lying vibrational modes of free canonical 2-deoxyribonucleosides	260 (2000)	317
Shizuka, H., see Moriyama, M.	253 (2000)	
Shobatake, K., see Kanda, K.	255 (2000)	
Shukla, A., see Abdurahman, A.	257 (2000)	
Shumay, I.L., see Fauster, T.	251 (2000)	111
Siegbahn, K., see Holland, D.M.P.	252 (2000)	257
Siegbahn, K., see Holland, D.M.P.	253 (2000)	
Siegbahn, K., see Potts, A.W.	254 (2000)	
Silvi, B., see Fuster, F.	252 (2000)	279
Simonson, J.M., see Chialvo, A.A.	258 (2000)	109

241110 1146.5 10 10141165 227 200	
Singer, K.D., see Ostroverkhov, V.	257 (2000) 263
Sjodin, T., CM. Li, H. Petek and HL. Dai, Ultrafast transient grating scattering	
studies of carrier dynamics at a silicon surface	251 (2000) 205
Skylaris, CK., see Gagliardi, L.	252 (2000) 47
Slone, R.V., see Vance, F.W.	253 (2000) 313
Smets, J., see Al-Jihad, I.	257 (2000) 167
Smets, J., see Smith, D.M.A.	260 (2000) 45
Smith, D.M.A., A.F. Jalbout, J. Smets and L. Adamowicz, Cytosine anions: ab initio	
study	260 (2000) 45
Smith, R.S., Z. Dohnálek, G.A. Kimmel, K.P. Stevenson and B.D. Kay, The self-	
diffusivity of amorphous solid water near 150 K	258 (2000) 291
Snavely, D.L., see Fedorov, A.V.	254 (2000) 169
Sobolewski, A.L. and W. Domcke, Conical intersections induced by repulsive ${}^{1}\pi\sigma^{*}$	
states in planar organic molecules: malonaldehyde, pyrrole and chlorobenzene as	
photochemical model systems	259 (2000) 181
Sohn, J., see Kim, S.	256 (2000) 289
Sokolov, N.D. and V.A. Savel'ev, Some regularities of vibrational spectra of a weak	
hydrogen bond: cooperative and 'anticooperative' effects within the framework of an	
electrostatic model	252 (2000) 393
Solà, M., see Forés, M.	260 (2000) 53
Soper, A.K., The radial distribution functions of water and ice from 220 to 673 K and	
at pressures up to 400 MPa	258 (2000) 121
Soudackov, A.V., see Vener, M.V.	254 (2000) 249
Soulard, P., see Asselin, P.	256 (2000) 195
Spalletti, A., see Marri, E.	260 (2000) 383
Spangenberg, D., see Schmitt, M.	254 (2000) 349
Spanget-Larsen, J., E.W. Thulstrup and J. Waluk, Electronic states of diphenyl- and	
dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical	
calculations	254 (2000) 135
Sprik, M., Computation of the p K of liquid water using coordination constraints	258 (2000) 139
Staemmler, V., see Urban, J.	255 (2000) 15
Stagira, S., M. Nisoli, S. De Silvestri, A. Stella, P. Tognini, P. Cheyssac and R. Kofman,	
Ultrafast optical relaxation dynamics in metallic nanoparticles: from bulk-like	
toward spatial confinement regime	251 (2000) 259
Stampfuß, P., see Mahapatra, S.	259 (2000) 211
Stampor, W., Electromodulation of fluorescence in hole-transporting materials (TPD,	
TAPC) for organic light-emitting diodes	256 (2000) 351
Starikov, E.B., Hartree-Fock crystal orbital calculation on sodium-intercalated	
fullerites $C_{60}Na_{10}$ and $C_{60}Na_{11}$	256 (2000) 149
Stass, D.V., see Toropov, Yu.V.	253 (2000) 231
Stedman, G.E., see Naguleswaran, S.	256 (2000) 207
Steer, R.P., see Hlady, J.C.	260 (2000) 249
Stella, A., see Stagira, S.	251 (2000) 259
Stepanić, V. and G. Baranović, Ground and excited states of isodiazene – an ab initio	254 (2000) 151
study	254 (2000) 151
Stern, C.L., see Vance, F.W.	253 (2000) 313
Stevenson, K.P., see Smith, R.S.	258 (2000) 291
Stock, G., see Hahn, S.	259 (2000) 297

Strasser, J., H.H.H. Homeier and H. Yersin, Triplet sublevels of metal organic	
complexes - temperature dependence of spin-lattice relaxation	255 (2000) 301
Suhai, S., see Elstner, M.	256 (2000) 15
Suhai, S., see Frimand, K.	255 (2000) 165
Sukhomlinova, L., see Ostroverkhov, V.	257 (2000) 263
Sumimoto, M., see Kimura, T.	253 (2000) 125
Sun, J., see Guan, D.	252 (2000) 179
Suzuki, C., J. Kawai, M. Takahashi, AM. Vlaicu, H. Adachi and T. Mukoyama, The	()
electronic structure of rare-earth oxides in the creation of the core hole	253 (2000) 27
Suzuki, I.H. and N. Saito, Energy dependences of fragment ion yields from acetone	()
photoexcited in the C1s and O1s transition regions	253 (2000) 351
Suzuki, T., see Goworek, T.	255 (2000) 347
Sviridenko, F.B., see Toropov, Yu.V.	253 (2000) 231
Svishchev, I.M., A.Yu. Zassetsky and P.G. Kusalik, Solvation structures in three	200 (2000) 201
dimensions	258 (2000) 181
	200 (2000) 101
Tabayashi, K., see Kanda, K.	255 (2000) 369
Tachibana, M. and K. Yoshizawa, Vibronic interactions in {6} and {18}hetero(A,B)	
annulenes	260 (2000) 303
Takahashi, M., see Ogi, Y.	255 (2000) 379
Takahashi, M., see Suzuki, C.	253 (2000) 27
Takayanagi, T., see Umemoto, H.	259 (2000) 39
Takeshima, M., see Fukuhara, M.	258 (2000) 97
Tan, Z., see Zhang, S.	255 (2000) 397
Tan, Z., see Zhang, Y.	252 (2000) 191
Tanaka, K., see Umemoto, H.	259 (2000) 39
Tang, BY., see Cai, MQ.	255 (2000) 283
Tang, BY., see Cai, MQ.	260 (2000) 281
Taylor, A.J., see Lobad, A.I.	251 (2000) 227
Terada, N., see Umemoto, H.	259 (2000) 39
Theodorakopoulos, G., see Petsalakis, I.D.	254 (2000) 181
Thiébault, A., see Combellas, C.	252 (2000) 165
Thomas, S.E., see Wilsey, S.	258 (2000) 21
Thulstrup, E.W., see Spanget-Larsen, J.	254 (2000) 135
Tkachenko, N.V., see Glebov, E.M.	257 (2000) 79
Tobita, S., see Moriyama, M.	253 (2000) 91
Tognini, P., see Stagira, S.	251 (2000) 259
Tokumoto, M., see Umek, P.	253 (2000) 361
Tolkachev, V.A., see Gelin, M.F.	255 (2000) 111
Tolosa, S., A. Hidalgo and J.A. Sansón, Thermodynamic, structural, and dynamic	
study of the N-H···O=C hydrogen bond association in aqueous solution	255 (2000) 73
Tom, H.W.K., see Chang, YM.	251 (2000) 283
Tomellini, M., see Molinari, E.	253 (2000) 367
Tong, J., see Li, XY.	260 (2000) 283
Torga, J.R., M.C. Marconi, R. Martín Negri and P.F. Aramendía, Molecular	
rotational diffusion detected by differential fluorescence energy	253 (2000) 249
Toropov, Yu.V., F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin,	
Influence of geminate recombination kinetics on the shape of low field MARY line	253 (2000) 231

28	Author index to volumes 251-200	
Treml. H. and HH. Kohler, Coupling	ng of diffusion and reaction in the process of	
capillary formation in alginate gel	1	252 (2000) 199
Troe, J., see Sander, M.U.		258 (2000) 257
Tronc, M., R. Azria, Y. Le Coat,	P. Cloutier and L. Sanche, Kinetic energy CO* produced by electron stimulated desorption	()
from condensed CO ₂		254 (2000) 69
Trudell, M.L., see Galasso, V.		254 (2000) 375
Trugman, S.A., see Lobad, A.I.		251 (2000) 227
	mid, Conical intersections, pseudorotation and	
	otodissociation of group-6 metal hexacarbonyls	259 (2000) 313
Tsukerblat, B.S., see Borras-Almenar,	J.J.	254 (2000) 275
Tsukerblat, B.S., see Palii, A.V.		255 (2000) 51
Tsukiyama, K., see Ogi, Y.		255 (2000) 379
Tucceri, M.E., see Badenes, M.P.		253 (2000) 205
Tuckerman, M.E., see Yarne, D.A.		258 (2000) 163
Tully, J.C., see LaBerge, L.J.		260 (2000) 183
Tunkin, V.G., see Kuznetsov, D.S.		257 (2000) 117
Turci, C.C., see Eustatiu, I.G.		257 (2000) 235
the geometrical dependence of deut	O.M. Harris, Systematic computational study of derium quadrupole interaction parameters in an	
O-2H···O=C hydrogen bonded sys	tem	256 (2000) 159
Twieg, R.J., see Ostroverkhov, V.		257 (2000) 263
Tyliszczak, T., see Eustatiu, I.G.		257 (2000) 235
Tyutyulkov, N., F. Dietz and K. M.	füllen, Magnetic exchange interaction between	
π -electron radicals adsorbed on gra	phites	255 (2000) 223
characterisation of fullerene deriva aminophenyl)-1H-methanofullerene Umemoto, H., N. Terada, K. Tanaka,	\acute{c} and M. Tokumoto, Synthesis and magnetic ative based ferromagnets 1-(3-nitro)- and 1-(3-doped with cobaltocene T. Takayanagi, Y. Kurosaki and K. Yokoyama, in the reactions of NO(A ² Σ ⁺) with C ₂ H ₂ , C ₂ H ₄ ,	253 (2000) 361
H ₂ O, and their isotopic variants		259 (2000) 39
Unamuno, Iñ., see Longarte, A.		260 (2000) 83
	and V. Staemmler, Ground and excited states of	
the Ne ₃ ⁺ molecule		255 (2000) 15
Usov, O.M., see Bagryansky, V.A.		255 (2000) 237
Valiron, P., see Faure, A.		254 (2000) 49
Vallée, R, see Del Fatti, N.		251 (2000) 215
	. Bakker, Observation of a bottleneck in the	, , , , ,
vibrational relaxation of liquid bro		253 (2000) 157
	ol of currents in semiconductors: a materials	
perspective		251 (2000) 309
van Emmichoven, P.A.Z., see Kok, A		258 (2000) 47
van Mourik, F., see Christophorov, L		256 (2000) 45
electroabsorption and electrochem	ern and J.T. Hupp, Comparative absorption, ical studies of intervalence electron transfer and	
electronic coupling in cyanide-brid	ged bimetallic systems: ancillary ligand effects	253 (2000) 313

9 5 7

Varandas, A.J.C. and Z.R. Xu, Singularities in the Hamiltonian at electronic	250 (2000) 153
degeneracies	259 (2000) 173
Varret, F., see Klokishner, S.	255 (2000) 317
Velegrakis, M., see Froudakis, G.E.	258 (2000) 13
Vener, M.V., I.V. Rostov, A.V. Soudackov and M.V. Basilevsky, Semiempirical	254 (2000) 240
modeling free energy surfaces for proton transfer in polar aprotic solvents	254 (2000) 249
Vetoshkin, E.V., see Benderskii, V.A.	257 (2000) 203
Vieil, E., see Miomandre, F.	255 (2000) 291
Vilaseca, E., see Madurga, S.	255 (2000) 123
Villani, G., see Ferretti, A.	259 (2000) 201
Vlaicu, AM., see Suzuki, C.	253 (2000) 27
Vogel, E., see Bock, S.	257 (2000) 147
Vold, R.L., see Kristensen, J.H.	252 (2000) 97
Voigt, A., U. Abram, R. Böttcher, U. Richter, J. Reinhold and R. Kirmse, Q-Band single-crystal EPR study and molecular orbital calculations of [(C ₆ H ₅) ₄ As][Re ^{VI} -	
NCl ₄ /Re ^V OCl ₄]	253 (2000) 171
Volk, M., see Kholodenko, Y.	259 (2000) 71
von Niessen, W., see Holland, D.M.P.	252 (2000) 257
von Niessen, W., see Holland, D.M.P.	253 (2000) 133
von Niessen, W., see Potts, A.W.	254 (2000) 385
Voth, G.A., see Čuma, M.	258 (2000) 187
Wolasfer C.F. and V.C. Chu Natura of military materials for the second state of the se	
Walrafen, G.E. and YC. Chu, Nature of collagen-water hydration forces: a problem in water structure	250 (2000) 427
Waluk, J., see Spanget-Larsen, J.	258 (2000) 427
Wang, B., see Hou, H.	254 (2000) 135
Wang, SX., see Ostroverkhov, V.	252 (2000) 17
Wang, T., see Zheng, N.W.	257 (2000) 263
Wang, X., see Chen, M.	258 (2000) 37 255 (2000) 95
Wang, X., see Kushto, G.P.	257 (2000) 223
Wang, X., see Zhang, L.	254 (2000) 231
Warns, Ch., see Barvík, I.	255 (2000) 403
Wasylyshyn, D.A., see McAnanama, J.G.	252 (2000) 237
Watson, F.H., see Evans, C.M.	260 (2000) 225
Weber, J., see Boulet, P.	253 (2000) 391
Wegener, M. and D.S. Chemla, Coherent control of electron-phonon quantum	
kinetics: exploring the weak and the strong coupling regime	251 (2000) 269
Weida, M.J., see Petek, H.	251 (2000) 71
Weinelt, M., see Fauster, T.	251 (2000) 111
Weitzel, KM., see Korolkov, M.V.	252 (2000) 209
Wellershoff, SS., see Hohlfeld, J.	251 (2000) 237
Wenzel, W., see Mahapatra, S.	259 (2000) 211
Westphal, A., see Schmitt, M.	254 (2000) 349
Wieczorek, R., see Kozłowski, M.	252 (2000) 289
Wiesenfeld, L., see Faure, A.	254 (2000) 49
Willetts, A., see Gagliardi, L.	252 (2000) 47

Wilsey, S., S.E. Thomas and J.H.D. Eland, An experimental and theoretical study of	
the HNCO ⁺ ion	258 (2000) 21
Winger, R.H., see Pichler, A.	258 (2000) 391
Wolfsberg, M., see Fritzsche, S.	253 (2000) 283
Wolter, J.H., see Meskers, S.C.J.	260 (2000) 415
Wong, C.M., see Gaffney, K.J.	251 (2000) 99
Wormell, P., see Fischer, G.	257 (2000) 1
Woutersen, S., see Bakker, H.J.	258 (2000) 233
Wu, C.Y.R., see Chen, F.Z.	260 (2000) 215
Wu, G., A classical algebraic approach to the bend motion of acetylene: the formalism	
by two coupled cosets	252 (2000) 315
Würger, A., see Bordat, P.	258 (2000) 63
Wurth, W. and D. Menzel, Ultrafast electron dynamics at surfaces probed by resonant	
Auger spectroscopy	251 (2000) 141
Xantheas, S.S., Cooperativity and hydrogen bonding network in water clusters	258 (2000) 225
Xu, K.Z., see Zhang, C.F.	256 (2000) 275
Xu, L., see Chang, YM.	251 (2000) 283
Xu, Z.R., see Varandas, A.J.C.	259 (2000) 173
Yajima, S., see Nakayama, H.	253 (2000) 331
Yamaguchi, K., see Nakano, M.	252 (2000) 115
Yang, GW., see Cai, MQ.	255 (2000) 283
Yang, GW., see Cai, MQ.	260 (2000) 281
Yang, R., see Zheng, N.W.	258 (2000) 37
Yarne, D.A., M.E. Tuckerman and M.L. Klein, Structural and dynamical behavior of	250 (2000) 162
an azide anion in water from ab initio molecular dynamics calculations	258 (2000) 163
Yersin, H., see Strasser, J.	255 (2000) 301
Yezdimer, E., see Chialvo, A.A.	258 (2000) 109
Yi, X., see Guan, D.	252 (2000) 179
Yi, X., see Zheng, Y.	255 (2000) 273
Yokoyama, K., see Umemoto, H.	259 (2000) 39
Yoshizawa, K., see Tachibana, M.	260 (2000) 303
You, XZ., see Zhu, XL.	253 (2000) 241
You, XZ., see Zhu, XL.	254 (2000) 287
Yu, Z., see Zhu, XL.	253 (2000) 241
Yuan, Z.S., see Zhang, C.F.	256 (2000) 275
Yurkovskaya, A.V., see Popov, A.V.	252 (2000) 83
Zaldo, C., see Cascales, C.	257 (2000) 29
Zanchini, C., Silylcyanides and silylisocyanides: a comparative theoretical study Zarić, S.D., Theoretical study of cation– π interactions of the metal complex cation,	254 (2000) 187
$[Co(NH_3)_6]^{3+}$, with ethylene and acetylene	256 (2000) 213
Zassetsky, A.Yu., see Svishchev, I.M.	258 (2000) 181
Zeegers-Huyskens, T., see Chandra, A.K.	255 (2000) 149
Zhang, C.F., X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu, Density functional theory	
studies of methylated uracil: geometries and energies	256 (2000) 275
Zhang, H., see Humbs, W.	254 (2000) 319

	51
Zhang, H., see Zhang, S.	255 (2000) 397
Zhang, H., see Zhang, Y.	252 (2000) 191
Zhang, J.Z.H., see Zhang, S.	255 (2000) 397
Zhang, J.Z.H., see Zhang, Y.	252 (2000) 191
Zhang, L. and M. Zhou, Theoretical investigation on the potential energy surface for	
the reactions of B, Al and Ga with NO	256 (2000) 185
Zhang, L., see Cai, MQ.	255 (2000) 283
Zhang, L., see Cai, MQ.	260 (2000) 281
Zhang, L., see Chen, M.	255 (2000) 95
Zhang, L., X. Wang, M. Chen and QZ. Qin, Activation of CO ₂ by Zr atom. Matrix-	
isolation FTIR spectroscopy and density functional studies	254 (2000) 231
Zhang, Q., see Zhang, Y.	252 (2000) 191
Zhang, S., Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang, Reactant-product	
decoupling approach to state-to-state reactive scattering H + DH	255 (2000) 397
Zhang, Y., see Zhang, S.	255 (2000) 397
Zhang, Y., see Zhu, XL.	254 (2000) 287
Zhang, Y., Z. Tan, H. Zhang, Q. Zhang and J.Z.H. Zhang, Time-dependent quantum dynamics study of reactive scattering of the HD+CN system in the potential	
averaged 5D model	252 (2000) 191
Zhang, Z.J., see Zhang, C.F.	256 (2000) 275
Zheng, N.W., T. Zhou, R. Yang, T. Wang and D. Ma, Analysis of the bound odd-parity spectrum of krypton by weakest bound electron potential model	
theory	258 (2000) 37
Zheng, Q., see Chen, M.	255 (2000) 95
Zheng, Y. and S. Ding, Algebraic approach to the potential energy surface for the electronic ground state of ozone	255 (2000) 217
Zheng, Y., see Feng, R.	255 (2000) 217
Zheng, Y., see Guan, D.	260 (2000) 29
Zheng, Y., see Litvinyuk, I.V.	252 (2000) 179
Zheng, Y., X. Yi, D. Guan and Q. Meng, Statistical dynamics in rotationally inelastic	253 (2000) 41
gas-surface scattering: dynamical Lie algebraic method	255 (2000) 273
Zhong, Y., see Zhu, XL.	253 (2000) 241
Zhou, M., see Zhang, L.	256 (2000) 185
Zhou, T., see Zheng, N.W.	258 (2000) 37
Zhu, XL., XZ. You and Y. Zhang, A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band	
theory	254 (2000) 287
Zhu, XL., XZ. You, Y. Zhong, Z. Yu and SL. Guo, An improved calculation	
method on optical second-order susceptibilities of organic materials	253 (2000) 241
Ziemniak, E., see Carvajal, M.	260 (2000) 105
Zilberg, S. and Y. Haas, Conical intersections in molecular photochemistry – the role of phase change	259 (2000) 249
Zilberg, S., see Fuß, W.	259 (2000) 273
Zitto, M.E., M.C. Caputo, M.B. Ferraro and P. Lazzeretti, Thomas-Reiche-Khun populations in X-CH ₃ and X-C ₂ H ₅ series of molecules	
Zubarev, V., see Goez, M.	
Zuppiroli, L., see Miomandre, F.	256 (2000) 107
Eupphon, L., see Mioinandie, F.	255 (2000) 291





Chemical Physics 251-260 (2000) 33-101

Chemical Physics

www.elsevier.nl/locate/chemphys

Subject index to volumes 251-260

Methods and constructs

Theoretical

Computational methods for electronic structure		
Electronic and structural properties of CaH ₂ : an ab initio Hartree-Fock study, A. El		
Gridani and M. El Mouhtadi	252 (2000)	1
Determination of protonation sites in bases from topological rules, F. Fuster and		
B. Silvi	252 (2000) 2	279
Dielectric relaxation and molecular conformational energy of some arylazo benzothia- zine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and		
A. Jurlewicz	252 (2000) 2	289
Some regularities of vibrational spectra of a weak hydrogen bond: cooperative and 'anticooperative' effects within the framework of an electrostatic model, N.D.		
Sokolov and V.A. Savel'ev	252 (2000) 3	393
The electron localization function description of aromaticity in five-membered rings, D.B. Chesnut and L.J. Bartolotti	253 (2000)	1
The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical study		
using combined discrete/self-consistent reaction field models, C. Alemán	253 (2000)	13
A universal Gaussian basis set for positive and negative ions from H through Xe, F.E.	, , ,	
Jorge and M.L. Franco	253 (2000)	21
The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,		
J. Kawai, M. Takahashi, AM. Vlaicu, H. Adachi and T. Mukoyama	253 (2000)	27
Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V.		
Litvinyuk, Y. Zheng and C.E. Brion	253 (2000)	4
Vibronic coupling for H ₂ CO and CO ₂ , A.B. Rocha and C.E. Bielschowsky	253 (2000)	5
Ab initio determination of the C ₆ H ₆ ···CS ₂ cluster stabilization energy, N.P. da	, ,	
Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto	253 (2000)	16:
Q-Band single-crystal EPR study and molecular orbital calculations of [(C ₆ H ₅) ₄ As]-[Re ^{VI} NCl ₄ /Re ^V OCl ₄], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and	,	
R. Kirmse	253 (2000)	17
A density functional study of H ₂ O-OClO, (H ₂ O) ₂ -OClO and H ₂ O-ClOO complexes,		
S. Aloisio and J.S. Francisco	254 (2000)	

·		
Ab initio study of $M(CH_3CN)_n$ clusters $(M = Li^+, Na^+, Mg^{2^+})$ in the gas phase, E.M.	254 (2000)	11
Cabaleiro-Lago and M.A. Ríos Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	254 (2000)	11
 Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the CO₂ + H₂ → HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud- 	254 (2000)	25
Dandine and A. Sevin	254 (2000)	99
The study of A(CH ₃ OH) ₁₋₆ (A = Li ⁺ , Na ⁺) in the gas phase based on ab initio calculations, analysis of the solvation process, A. García-Muruais, E.M. Cabaleiro-Lago, J.M. Hermida-Ramón and M.A. Ríos	254 (2000)	109
Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova		
and S. Peyerimhoff Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular	254 (2000)	123
dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	0.5.1 (0.000)	107
and J. Waluk Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G.	254 (2000)	135
Baranović	254 (2000)	151
Direct correlation method for OH, NH and CH local modes: vibrational overtone spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylene-		
diamine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000)	
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000)	187
Structural properties and quantum effects in protonated helium clusters. I. The ab initio	254 (2000)	202
interaction potential, B. Balta and F.A. Gianturco	254 (2000)	203
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S. Karabunarliev and M. Baumgarten	254 (2000)	230
Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-	254 (2000)	437
dichloropropane in carbon tetrachloride, S. Madurga, J.C. Paniagua and E. Vilaseca	255 (2000)	123
Infrared spectra of monomeric L-alanine and L-alanine-N-d ₃ zwitterions isolated in a KBr matrix, X. Cao and G. Fischer	255 (2000)	105
DFT studies on helix formation in N -acetyl- $(L$ -alanyl) $_n$ - N' -methylamide for $n = 1-20$, M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and	255 (2000)	193
S. Suhai	256 (2000)	15
Hartree–Fock crystal orbital calculation on sodium-intercalated fullerites C ₆₀ Na ₁₀ and	200 (2000)	
C ₆₀ Na ₁₁ , E.B. Starikov	256 (2000)	149
Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $O^{-2}H\cdots O=C$ hydrogen bonded system, G.W.		
Turner, R.L. Johnston and K.D.M. Harris	256 (2000)	159
New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski	256 (2000)	177
Theoretical study of cation– π interactions of the metal complex cation, $[Co(NH_3)_6]^{3+}$,	230 (2000)	1//
with ethylene and acetylene, S.D. Zarić	256 (2000)	213
Vibronic analyses of the lowest singlet-singlet and singlet-triplet band systems of pyridazine, G. Fischer and P. Wormell	257 (2000)	1
A comparison of the oxygen 1s photoabsorption spectra of SO ₂ and NO ₂ , A. Jürgensen and R.G. Cavell	257 (2000)	123
The pair density description of aromaticity in some substituted cyclopentadienyl	257 (2500)	
systems: a comparison of AIM and ELF bonding descriptors, D.B. Chesnut and L.J. Bartolotti	257 (2000)	175
AND AND TOTAL	237 (2000)	110

alculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of configuration interaction methods, S. Lacombe, M. Loudet,	
A. Dargelos and J.M. Camou Mass spectra and theoretical modeling of Li^+Ne_n , Li^+Ar_n and Li^+Kr_n clusters, G.E.	258 (2000) 1
Froudakis, S.C. Farantos and M. Velegrakis	258 (2000) 13
theoretical study on a Diels-Alder reaction in ambient and supercritical water:	
viewing solvent effects through frontier orbitals, Y. Harano, H. Sato and F. Hirata	258 (2000) 151
Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Chomas–Reiche–Khun populations in $X-CH_3$ and $X-C_2H_5$ series of molecules, M.E.	258 (2000) 225
Zitto, M.C. Caputo, M.B. Ferraro and P. Lazzeretti ab initio study of the reaction mechanism of singlet and triplet N ₂ O and their	259 (2000) 1
intersystem crossing, DY. Hwang and A.M. Mebel	259 (2000) 89
Conical intersections and photoreactions of 2H-azirines, C. Bornemann and M.	
Klessinger Vibrational corrections to linear and nonlinear static electric properties of polyatomic	259 (2000) 263
molecules at non-optimum reference geometry, V.E. Ingamells, M.G. Papadopoulos	2(0 (2000) 1
and A.J. Sadlej On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, O. Plashkevych, T. Privalov,	260 (2000) 1
H. Ågren, V. Carravetta and K. Ruud	260 (2000) 11
Orbital imaging for the valence shell of sulphur dioxide: comparison of EMS measurements with near Hartree-Fock limit and density functional theory, R. Feng,	
Y. Sakai, Y. Zheng, G. Cooper and C.E. Brion Ab initio calculation for inner reorganization energy of gas-phase electron transfer in	260 (2000) 29
organic molecule-ion systems, XY. Li, J. Tong and FC. He	260 (2000) 283
CI and valence bond approach	
Theoretical spectroscopic data of the HO ₂ ⁺ ion, J.M. Robbe, M. Monnerville, G. Chambaud, P. Rosmus and P.J. Knowles	252 (2000) 9
Vibronic coupling for H ₂ CO and CO ₂ , A.B. Rocha and C.E. Bielschowsky	253 (2000) 51
Electronic states of CF ⁺ , I.D. Petsalakis and G. Theodorakopoulos	254 (2000) 181
Study of electron polarization and correlation effects in resonant and background	255 (2000) 1
electron scattering off CF ₃ Cl, T. Beyer, B.M. Nestmann and S.D. Peyerimhoff The nuclear spin-spin coupling constants in methanol and methylamine: geometry and	255 (2000)
solvent effects, M. Pecul and J. Sadlej Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species,	255 (2000) 137
N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews	255 (2000) 205
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M.	
Aubert-Frécon	256 (2000) 1
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, DY. Hwang and A.M. Mebel	256 (2000) 169
Ab initio calculations of the electronic states of KRb, S.J. Park, Y.J. Choi, Y.S. Lee and GH. Jeung	257 (2000) 135
An experimental and theoretical study of the HNCO ⁺ ion, S. Wilsey, S.E. Thomas and J.H.D. Eland	258 (2000) 21

-perturbative and many body approaches The rest of including lifetimes of law energy electrons in metals B.M. Februines I.M.		
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M. Pitarke, E.V. Chulkov and A. Rubio	251 (2000)	1
The attractive quartet potential energy surface for the $CH_3C(a^4A_2) + CO$ reaction, H.	231 (2000)	1
Hou, B. Wang and Y. Gu	252 (2000)	17
Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of		
the transitions probability from metastable states., B.F. Minaev	252 (2000)	25
Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene	252 (2000)	50
and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar Nuclear quadrupole coupling constant of ²¹ Ne in the neon dimer and its influence on	253 (2000)	39
the T_1 NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and		
M. Jaszuński	253 (2000)	183
Ground and excited states of the Ne ₃ ⁺ molecule, J. Urban, P. Mach, J. Mášik, I. Hubač		
and V. Staemmler	255 (2000)	15
Theoretical study of the infrared and ultraviolet spectrum of the radical F ₂ CN, H. Dupin, I. Baraille, C. Larrieu and A. Dargelos	256 (2000)	7
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, DY.	230 (2000)	/
Hwang and A.M. Mebel	256 (2000)	169
New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by		
H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski	256 (2000)	177
A new intermolecular potential energy surface for carbon dioxide from ab initio	257 (2000)	147
calculations, S. Bock, E. Bich and E. Vogel Ab initio study of the $F_2(X^1\Sigma_{\sigma}^+)$ – $H(^2S)$ van der Waals complex, V. Lukeš, M.	257 (2000)	14/
Bittererová, V. Laurinc and S. Biskupič	257 (2000)	157
Isomerism of the covalent anion of the dimer of uracil and 1-methyl-cytosine: ab initio		
study, I. Al-Jihad, J. Smets and L. Adamowicz	257 (2000)	167
Correlated ground-state ab initio calculations of polymethineimine, A. Abdurahman,	257 (2000)	201
A. Shukla and M. Dolg Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas	257 (2000) 258 (2000)	
Topological effects in molecular systems: an attempt towards a complete theory, M. Baer	259 (2000)	
Conical intersections induced by repulsive ${}^{1}\pi\sigma^{*}$ states in planar organic molecules:	()	
malonaldehyde, pyrrole and chlorobenzene as photochemical model systems, A.L.		
Sobolewski and W. Domcke	259 (2000)	181
Cytosine anions: ab initio study, D.M.A. Smith, A.F. Jalbout, J. Smets and L. Adamowicz	260 (2000)	15
Substituent effects on the intramolecular proton transfer in the ground and lowest-lying	200 (2000)	40
singlet excited states of salicylaldimine, M. Forés, M. Duran and M. Solà	260 (2000)	53
The equilibrium N-H bond length, J. Demaison, L. Margulès and J.E. Boggs	260 (2000)	65
Vertical triple ionization of ethyne molecules in triple-electron-transfer collisions with		
O ²⁺ beam ions, N. Jeffreys, D.E. Parry and F.M. Harris	260 (2000)	295
-density functional theory		
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M.		
Pitarke, E.V. Chulkov and A. Rubio	251 (2000)	1
A theoretical study of plutonium diketone complexes for solvent extraction, L.	252 (2000)	47
Gagliardi, N.C. Handy, CK. Skylaris and A. Willetts DFT and HF-DFT calculations of ¹⁴ N quadrupole coupling constants in molecules,	252 (2000)	4/
W.C. Bailey	252 (2000)	57
	(====)	- /

Diagret mass to commes 251 200		21
Density functional study of electronic, magnetic and hyperfine properties of [M(CN) ₅ -		
NO^{2-} (M = Fe, Ru) and reduction products, J.A. Gómez and D. Guenzburger Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman	253 (2000)	73
and computational study, A. Kovács, G. Keresztury and V. Izvekov Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E.	253 (2000) 1	93
Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri	253 (2000) 2	205
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000) 1	87
Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco	254 (2000) 2	203
Activation of CO ₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin	254 (2000) 2	231
Density functional calculations on simple carbonyl bases: protonation and hydrogen	, , ,	
bond formation with water, A.K. Chandra, M.T. Nguyen and T. Zeegers-Huyskens Structures, vibrational absorption and vibrational circular dichroism spectra of Lalanine in aqueous solution: a density functional theory and RHF study, K.	255 (2000) 1	149
Frimand, H. Bohr, K.J. Jalkanen and S. Suhai	255 (2000) 1	165
Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species,		
N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews	255 (2000) 2	205
DFT studies on helix formation in N-acetyl-(L-alanyl) _n -N'-methylamide for $n = 1-20$,		
M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, DY.	256 (2000)	
Hwang and A.M. Mebel	256 (2000)	169
Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou	256 (2000)	185
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E.		
Alikhani and J.P. Perchard	256 (2000)	195
Density functional theory studies of methylated uracil: geometries and energies, C.F.	257 (2000)	275
Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu Theoretical study on the conduith dusters of No. (COT) by density functional	256 (2000)	213
Theoretical study on the sandwich clusters of $Na_n(COT)_m$ by density functional method, JG. Han, WM. Pang and YY. Shi	257 (2000)	21
The pair density description of aromaticity in some substituted cyclopentadienyl systems: a comparison of AIM and ELF bonding descriptors, D.B. Chesnut and L.J.	257 (2000)	21
Bartolotti	257 (2000)	175
Computation of the pK of liquid water using coordination constraints, M. Sprik	258 (2000)	
Structural and dynamical behavior of an azide anion in water from ab initio molecular		
dynamics calculations, D.A. Yarne, M.E. Tuckerman and M.L. Klein	258 (2000)	163
The equilibrium N-H bond length, J. Demaison, L. Margulès and J.E. Boggs	260 (2000)	65
Structure and ground and first electronic excited state vibrational modes of the ethyl-p-aminobenzoate conformers, A. Longarte, J.A. Fernández, I. Unamuno and F.		
Castaño	260 (2000)	83
Vibronic interactions in {6} and {18}hetero(A,B)annulenes, M. Tachibana and K. Yoshizawa	260 (2000)	303
Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonucleosides, O.V. Shishkin, A. Pelmenschikov, D.M. Hovorun and J. Leszczynski	260 (2000)	317
Density functional theory and Hartree–Fock-density functional theory calculations of ¹⁷ O, ³³ S, and ⁷³ Ge quadrupole coupling constants, W.C. Bailey, F.M. Gonzalez and		
J. Castiglione	260 (2000)	327

G.-H. Jeung

Semiempirical methods	
Dielectric relaxation and molecular conformational energy of some arylazo benzothia- zine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and A.	
Jurlewicz	252 (2000) 289
Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin	252 (2000) 301
Excited-state intramolecular proton transfer followed by <i>cis-trans</i> isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and	
H. Shizuka	253 (2000) 91
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S. Karabunarliev and M. Baumgarten	254 (2000) 239
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
DFT studies on helix formation in N -acetyl- $(L$ -alanyl) $_n$ - N' -methylamide for $n = 1-20$, M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S.	
Suhai	256 (2000) 15
Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclote-tradecane)chromium(III) nitrate, JH. Choi	256 (2000) 29
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J.	
Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
Optical spectroscopy and crystal-field effects on the paramagnetic susceptibility of rare- earth germanates GaRGe ₂ O ₇ , R = Pr, Nd, C. Cascales, G. Lozano, C. Zaldo and P.	
Porcher	257 (2000) 29
Analysis of the bound odd-parity spectrum of krypton by weakest bound electron	
potential model theory, N.W. Zheng, T. Zhou, R. Yang, T. Wang and D. Ma	258 (2000) 37
Semi-empirical study of chain conformation and absorption spectra of polyanilines:	
size, solvent and disorder effects, Z.T. de Oliveira and M.C. dos Santos	260 (2000) 95
A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae	260 (2000) 337
A STATE OF THE STA	, , , , , , , , , , , , , , , , , , , ,
Algebraic approaches	
A classical algebraic approach to the bend motion of acetylene: the formalism by two	
coupled cosets, G. Wu	252 (2000) 315
Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler, E.E.	
	areas as a selection of the

Gooch, J.L. Dial and S.K. Knudson	253 (2000) 219	
Algebraic approach to the potential energy surface for the electronic ground state of	200 (2000) 217	
ozone, Y. Zheng and S. Ding	255 (2000) 217	
An extended SU(2) model for coupled Morse oscillators, M. Carvajal, R. Lemus, A.		
Frank, C. Jung and E. Ziemniak	260 (2000) 105	
Relativistic electronic structure theory		
A theoretical study of plutonium diketone complexes for solvent extraction, L. Gagliardi, N.C. Handy, CK. Skylaris and A. Willetts	252 (2000) 47	
Ab initio calculations of the electronic states of KRb, S.J. Park, Y.J. Choi, Y.S. Lee and		

257 (2000) 135

Wavefunctions for highly excited and unbound states		
Gaussian Type Orbitals basis sets for the calculation of continuum properties in molecules: the differential photoionization cross section of acetylene, I. Cacelli, R.		
Moccia and A. Rizzo Ab initio calculations of the electronic states of KRb, S.J. Park, Y.J. Choi, Y.S. Lee and	252 (2000)	67
GH. Jeung	257 (2000)	135
Calculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of configuration interaction methods, S. Lacombe, M. Loudet, A. Dargelos and J.M. Camou	258 (2000)	
Spin states and magnetic interactions		
Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of		
the transitions probability from metastable states, B.F. Minaev	252 (2000)	25
Calculation of CIDNP field dependences in biradicals in the photolysis of large-ring		
cycloalkanones, A.V. Popov, P.A. Purtov and A.V. Yurkovskaya	252 (2000)	83
Motional effects on optimum coherence transfer in ² H MAS NMR spectroscopy, J.H.	252 (2000)	
Kristensen, G.L. Hoatson and R.L. Vold	252 (2000)	97
Density functional study of electronic, magnetic and hyperfine properties of $[M(CN)_5NO]^{2-}$ (M = Fe, Ru) and reduction products, J.A. Gómez and D.		
$[M(CN)_5NO]$ (M = Fe, Ru) and reduction products, J.A. Gomez and D. Guenzburger	253 (2000)	72
Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis	233 (2000)	13
and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M.		
Maggini, M. Prato, I. Lamparth and A. Hirsch	253 (2000)	105
Influence of geminate recombination kinetics on the shape of low field MARY line,	200 (2000)	200
Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin	253 (2000)	231
Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,		
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000)	25
Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras-		
Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat	254 (2000)	275
Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with high-		
spin $S = 3/2$ ground state, M.I. Belinsky	255 (2000)	23
Vibronic model of hyperfine interaction in dimeric mixed-valence clusters, A.V. Palii,	255 (2000)	
M.I. Belinsky and B.S. Tsukerblat	255 (2000)) 51
Magnetic exchange interaction between π -electron radicals adsorbed on graphites, N. Tyutyulkov, F. Dietz and K. Müllen	255 (2000)	222
Quantum beats in recombination of spin-correlated radical ion pairs with equivalent	255 (2000)) 443
protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N.		
Molin	255 (2000)	237
Li cation–aromatic organic radical complex in a zeolite studied by electron spin echo	200 (2000)	, 20,
envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W.		
Dwyer	256 (2000)	37
Recombination yield of geminate radical pairs in high magnetic fields: general results		
and application to free diffusion, M.J. Hansen, A.A. Neufeld and J.B. Pedersen	260 (2000)	125
Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolar-		
izabilities)		
Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanopar-		
ticles, T.V. Shahbazyan and I.E. Perakis	251 (2000)) 37

Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of the transitions probability from metastable states, B.F. Minaev Electron-photon field dynamics: numerically exact calculations of multi-state molecule	252 (2000) 25
systems interacting with a single-mode coherent photon field, M. Nakano and K. Yamaguchi Molecular motions in molecular glasses as studied by thermally stimulated depolarisa-	252 (2000) 115
tion currents (TSDC), N.T. Correia, C. Alvarez, J.J. Moura Ramos and M. Descamps	252 (2000) 151
Zwitterionic polymers for nonlinear optics, C. Combellas, F. Kajzar, G. Mathey, M.A. Petit and A. Thiébault	252 (2000) 165
An improved calculation method on optical second-order susceptibilities of organic materials, XL. Zhu, XZ. You, Y. Zhong, Z. Yu and SL. Guo	253 (2000) 241
Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martín Negri and P.F. Aramendía	253 (2000) 249
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band theory, XL. Zhu, XZ. You and Y.	254 (2000) 135
Zhang	254 (2000) 287
The nuclear spin-spin coupling constants in methanol and methylamine: geometry and solvent effects, M. Pecul and J. Sadlej	255 (2000) 137
Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy, N. Došlić and O. Kühn	255 (2000) 247
Dielectric relaxations of collagen and elastin in the dehydrated state, V. Samouillan, A. Lamure and C. Lacabanne	255 (2000) 259
Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J.	
Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho Electroabsorption spectroscopy of distyrylbenzene derivatives, P.A. Lane, H. Mellor,	256 (2000) 289
S.J. Martin, T.W. Hagler, A. Bleyer and D.D.C. Bradley Thomas–Reiche–Khin populations in X–CH ₃ and X–C ₂ H ₅ series of molecules, M.E.	257 (2000) 41
Zitto, M.C. Ceputo, M.B. Ferraro and P. Lazzeretti Vibrational corrections to linear and nonlinear static electric properties of polyatomic molecules at non-optimum reference geometry, V.E. Ingamells, M.G. Papadopoulos	259 (2000) 1
and A.J. Sadlej	260 (2000) 1
Radiative (incl. relativistic) effects on molecules and molecular processes Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of	
the transitions probability from metastable states., B.F. Minaev Gaussian Type Orbitals basis sets for the calculation of continuum properties in molecules: the differential photoionization cross section of acetylene, I. Cacelli, R.	252 (2000) 25
Moccia and A. Rizzo	252 (2000) 67

Smoles that to tolumes 201 200	41
Broadening and shifting coefficients of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure H ₂ : coupled states and semiclassical calculations. Comparison with experiments, X.	
Bruet, J. Bonamy and M.L. Dubernet-Tuckey Kinetic modelling of radiative reacting gas flow under strong nonequilibrium	254 (2000) 297
conditions, E.V. Kustova and A. Chikhaoui Prediction of pure electric-dipole two-photon absorption circular dichroism in	255 (2000) 59
lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
Topological effects in molecular systems: an attempt towards a complete theory, M. Baer	259 (2000) 123
Scattering of waves and particles	
Dynamical Lie algebraic approach to rotationally inelastic scattering of molecules from	
surfaces, D. Guan, X. Yi, Y. Zheng, S. Ding and J. Sun	252 (2000) 179
Broadening and shifting coefficients of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure	
H ₂ : coupled states and semiclassical calculations. Comparison with experiments, X.	
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Study of electron polarization and correlation effects in resonant and back- ground electron scattering off CF ₃ Cl, T. Beyer, B.M. Nestmann and S.D.	
Peyerimhoff	255 (2000) 1
Statistical dynamics in rotationally inelastic gas-surface scattering: dynamical Lie	255 (2000)
algebraic method, Y. Zheng, X. Yi, D. Guan and Q. Meng	255 (2000) 273
A recursive Kohn variational algorithm for the Green's operator: application to the	
T-matrix, D. Brown	259 (2000) 11
Topological effects in molecular systems: an attempt towards a complete theory, M.	
Baer	259 (2000) 123
Collisional and reactive molecular dynamics with non-frictional forces	
Time-dependent quantum dynamics study of reactive scattering of the HD + CN system	
in the potential averaged 5D model, Y. Zhang, Z. Tan, H. Zhang, Q. Zhang and	
J.Z.H. Zhang	252 (2000) 191
Relaxation of individual rotational levels of the \widetilde{A}^1A_u electronic state of acetylene	
excited to the $2v_3'$ and $(v_1' + v_3' + v_6')$ vibrational modes, V.I. Makarov and E. Quiñones	252 (2000) 250
Quasiclassical calculation of the chemical reaction Sr + HF, MQ. Cai, L. Zhang, BY.	253 (2000) 259
Tang, MD. Chen, GW. Yang and KL. Han	255 (2000) 283
Reactant-product decoupling approach to state-to-state reactive scattering H + DH, S.	233 (2000) 203
Zhang, Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang	255 (2000) 397
Quasi-classical dynamics and vibrational kinetics of $N + N_2(v)$ system, F. Esposito, M.	
Capitelli and C. Gorse	257 (2000) 193
State selected reactions of krypton ions with methane, A. Kok, P.A.Z. van	
Emmichoven and A. Niehaus	258 (2000) 47
Topological effects in molecular systems: an attempt towards a complete theory, M. Baer	250 (2000) 122
The geometric phase effect in chemical reactions, S. Adhikari and G.D. Billing	259 (2000) 123 259 (2000) 149
o i i i i i i i i i i i i i i i i i i i	-27 (2000) 117
Reactive molecular dynamics including dissipative processes	
Photodesorption of NO from a metal surface: quantum dynamical implications of a	
two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce	251 (2000) 51

Coupling of diffusion and reaction in the process of capillary formation in alginate gel, H. Treml and HH. Kohler	252 (2000) 199
Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and M.F. Gelin	252 (2000) 323
Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy, N. Došlić and O. Kühn	255 (2000) 247
Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik Quantum dynamics of model proton-coupled electron transfer reactions, S. Shin and S	256 (2000) 45
I. Cho	259 (2000) 27
Production processes of $H(D)$ atoms in the reactions of $NO(A^2\Sigma^+)$ with C_2H_2 , C_2H_4 , H_2O , and their isotopic variants, H . Umemoto, N . Terada, K . Tanaka, T .	
Takayanagi, Y. Kurosaki and K. Yokoyama Quasi-classical trajectory simulations of C + NO crossed molecular beam experiments,	259 (2000) 39
S. Andersson, N. Marković and G. Nyman Relaxation processes in singlet O ₂ analyzed by laser-induced gratings, W. Hubschmid	259 (2000) 99
and B. Hemmerling Photodissociation dynamics of CH ₂ BrCl at 234 nm, SH. Lee, YJ. Jung and KH.	259 (2000) 109
Jung	260 (2000) 143
Intramolecular dynamics	
The predissociation dynamics of vibrational eigenstates in the $A^2\Sigma^+$ state of HBr ⁺ ions: numerical solution of coupled time-dependent Schrödinger equations, M.V. Korolkov and KM. Weitzel	252 (2000) 209
A classical algebraic approach to the bend motion of acetylene: the formalism by two	232 (2000) 209
coupled cosets, G. Wu	252 (2000) 315
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination	
channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W. North Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	254 (2000) 309
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek Tunneling splittings in vibrational spectra of non-rigid molecules V.A. Benderskii and	254 (2000) 319
E.V. Vetoshkin	257 (2000) 203
The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1	207 (2000) 200
state of Cd-Ar, G.D. Roston and M.S. Helmi	258 (2000) 55
A theoretical study on a Diels-Alder reaction in ambient and supercritical water: viewing solvent effects through frontier orbitals, Y. Harano, H. Sato and F. Hirata Singularities in the Hamiltonian at electronic degeneracies, A.J.C. Varandas and Z.R.	258 (2000) 151
Xu	259 (2000) 173
Quantum and semiclassical dynamics of the Franck-Condon wave packet on the coupled potential surfaces of the $\tilde{X}^2A'/\tilde{A}^2A'$ conical intersection, F. Santoro, C.	200 (2000) 110
Petrongolo, G. Granucci and M. Persico	259 (2000) 193
A model study of the wavepacket dynamics around a Jahn-Teller conical intersection in a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani	250 (2000) 201
Nonadiabatic wave packet dynamics on the coupled $\tilde{X}^2A_1/\tilde{A}^2B_2$ electronic states of NO ₂ based on new ab initio potential energy surfaces, S. Mahapatra, H. Köppel,	259 (2000) 201
L.S. Cederbaum, P. Stampfuß and W. Wenzel Effect of a dissipative environment on the dynamics at a conical intersection, A. Kühl	259 (2000) 211
and W. Domcke	259 (2000) 227

Subject miles to comme 227 200	45
Conical intersections in molecular photochemistry – the role of phase change, S. Zilberg and Y. Haas	259 (2000) 249
Twin states and conical intersections in linear polyenes, W. Fuß, Y. Haas and S. Zilberg	259 (2000) 249
Femtosecond secondary emission arising from the nonadiabatic photoisomerization in rhodopsin, S. Hahn and G. Stock	259 (2000) 297
Impulsive IR-multiphoton dissociation of acrolein: observation of non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR fluorescence	
Spectroscopy, P.K. Chowdhury Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonu-	260 (2000) 151
cleosides, O.V. Shishkin, A. Pelmenschikov, D.M. Hovorun and J. Leszczynski	260 (2000) 317
Molecular dynamics of many particle systems and condensed phases	
Photodesorption of NO from a metal surface: quantum dynamical implications of a	251 (2000) 51
two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-	251 (2000) 51
Quraishi	252 (2000) 337
The solvent influence on the electrochemical transfer of divalent ions, O. Pecina and W.	232 (2000) 337
Schmickler	252 (2000) 349
Nuclear quadrupole coupling constant of ²¹ Ne in the neon dimer and its influence on	
the T_1 NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and	
M. Jaszuński	253 (2000) 183
Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman	253 (2000) 267
Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	
charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond	
association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón	255 (2000) 73
Mandelstam-Brillouin spectra and hyperacoustic velocities dispersion of trideuteroa-	
cetonitrile in the liquid state, R.S. Cataliotti, P. Sassi, A. Morresi and G. Paliani	255 (2000) 85
Theoretical study of cation– π interactions of the metal complex cation, $[Co(NH_3)_6]^{3+}$,	
with ethylene and acetylene, S.D. Zarić	256 (2000) 213
Determination of population, orientation and alignment of symmetric top molecule	256 (2000) 225
using laser-induced fluorescence, SL. Cong, KL. Han, GZ. He and NQ. Lou	256 (2000) 225
The isotopic and temperature dependent properties of hydrogen chloride dissolved in	257 (2000) 51
carbon tetrachloride. A molecular dynamics approach, G. Chatzis and J. Samios Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E.	257 (2000) 51
Froudakis, S.C. Farantos and M. Velegrakis	258 (2000) 13
The anomalous Stark effect of single terrylene molecules in <i>p</i> -terphenyl crystals, P.	238 (2000) 13
Bordat, M. Orrit, R. Brown and A. Würger	258 (2000) 63
The structure of water from 25°C to 457°C: comparison between neutron scattering and	200 (2000) 02
molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and	
J.M. Simonson	258 (2000) 109
The radial distribution functions of water and ice from 220 to 673 K and at pressures up	
to 400 MPa, A.K. Soper	258 (2000) 121
Computation of the pK of liquid water using coordination constraints, M. Sprik Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G.	258 (2000) 139
Kusalik	258 (2000) 181
A multi-state empirical valence bond model for acid-base chemistry in aqueous	
solution, M. Čuma, U.W. Schmitt and G.A. Voth	258 (2000) 187

Extent of inter-hydrogen bond correlations in water. Temperature effect, A. Luzar	258 (2000) 267
Slow dynamics in supercooled water, F. Sciortino	258 (2000) 307
A theoretical analysis of the sum frequency generation spectrum of the water surface, A. Morita and J.T. Hynes	258 (2000) 371
The role of water in B-DNAs B_I to B_{II} conformer substates interconversion: a combined	230 (2000) 371
study by calorimetry, FT-IR spectroscopy and computer simulation, A. Pichler, S.	
Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer	258 (2000) 391
Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt	258 (2000) 405
Intermolecular potential for benzoic acid—water based on the test-particle model and	200 (2000) 100
statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	
and B.M. Rode	260 (2000) 159
Quasiparticle dynamics (incl. excitons, polarons)	
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M.	
Pitarke, E.V. Chulkov and A. Rubio	251 (2000) 1
The role of Auger decay in hot electron excitation in copper, H. Petek, H. Nagano, M.J. Weida and S. Ogawa	251 (2000) 71
Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the	231 (2000) 71
distance estimation between trap sites, SG. Kang, WS. Chae, YR. Kim, JS.	
Jung and SH. Lee	256 (2000) 295
The lowest energy Frenkel and charge-transfer excitons in quasi-one-dimensional structures: application to MePTCDI and PTCDA crystals, M. Hoffmann, K.	
Schmidt, T. Fritz, T. Hasche, V.M. Agranovich and K. Leo	258 (2000) 73
Minutelian and interpreting an aride and leasting	
Migration and interaction on grids and lattices Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of	
lattice vibrations and of mutual interaction in the diffusion of methane in a cation-	
free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg	253 (2000) 283
Influence of the local electric field on ionic transport during redox switching of conducting polymers, F. Miomandre, M.N. Bussac, E. Vieil and L. Zuppiroli	255 (2000) 291
conducting polymers, F. Miomandre, M.N. Bussac, E. Vien and L. Zupphon	255 (2000) 291
Statistical computational methods (incl. Monte Carlo)	
Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri	252 (2000) 205
Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of	253 (2000) 205
lattice vibrations and of mutual interaction in the diffusion of methane in a cation-	
free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg	253 (2000) 283
A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp	253 (2000) 295
Monte Carlo simulation study of solvent effect on Na [†] to Li [†] ion mutation, HS. Kim	253 (2000) 305
Temperature dependence of fast neutral-neutral reactions: a triatomic model study,	
A. Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	
Paesani	254 (2000) 215
Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-	255 (2022) 122
dichloropropane in carbon tetrachloride, S. Madurga, J.C. Paniagua and E. Vilaseca	255 (2000) 123

)7

Subject times to totalies 251-200	43
Influence of the local electric field on ionic transport during redox switching of	
conducting polymers, F. Miomandre, M.N. Bussac, E. Vieil and L. Zuppiroli Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-	255 (2000) 291
level systems, S. Longo, D. Bruno and P. Minelli The isotopic and temperature dependent properties of hydrogen chloride dissolved in	256 (2000) 265
carbon tetrachloride. A molecular dynamics approach, G. Chatzis and J. Samios	257 (2000) 51
Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes New perspectives on hydrophobic effects, G. Hummer, S. Garde, A.E. García and L.R.	258 (2000) 201
Pratt	258 (2000) 349
Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt	258 (2000) 405
Eigenvalue spectrum of the survival probability of excitation in nonradiative energy transport, E.N. Bodunov, M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G.	238 (2000) 403
Martinho	259 (2000) 49
A rigorous procedure for combining molecular dynamics and Monte Carlo simulation	
algorithms, L.J. LaBerge and J.C. Tully	260 (2000) 183
Hopfield neural network model for calculating the potential energy function from	
second virial data, J.P. Braga, M.B. de Almeida, A.P. Braga and J.C. Belchior	260 (2000) 347
Dynamics of structures, lattices and macromolecular conformations	
Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	
H. Treml and HH. Kohler	252 (2000) 199
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low	254 (2000) 21
temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller Triplet sublevels of metal organic complexes – temperature dependence of spin–lattice	254 (2000) 31
relaxation, J. Strasser, H.H.H. Homeier and H. Yersin	255 (2000) 301
Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion	()
chambers, A.L. Itkin	256 (2000) 61
Fluctuations and random processes	
Stretched exponentials and barrier distributions, O. Edholm and C. Blomberg	252 (2000) 221
Some remarks on the application of relaxation techniques to chemical equilibria, M.	254 (2000) 220
Galán and G. Angulo	254 (2000) 329
Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik	256 (2000) 45
Non-equilibrium statistical mechanics	
Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in	
desorption, J.W. Gadzuk	251 (2000) 87
Stretched exponentials and barrier distributions, O. Edholm and C. Blomberg	252 (2000) 221
Self-diffusion in liquid metals, A.S. Chauhan, R. Ravi and R.P. Chhabra	252 (2000) 227
Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and	252 (2000) 222
M.F. Gelin	252 (2000) 323
Role of inertial and non-Markovian effects on activated barrier crossing dynamics for charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 20
A proper mobility formula for large, heavy particles in gases in any regime, L. Ferrari	254 (2000) 39 257 (2000) 63
Vibrational energy storage in high pressure mixtures of diatomic molecules, E. Plönjes,	
P. Palm, W. Lee, M.D. Chidley, I.V. Adamovich, W.R. Lempert and J.W. Rich	260 (2000) 353

Non-equilibrium thermodynamic and hydrodynamic theories	
Kinetic modelling of radiative reacting gas flow under strong nonequilibrium conditions, E.V. Kustova and A. Chikhaoui	255 (2000) 59
Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion	255 (2000) 59
chambers, A.L. Itkin	256 (2000) 61
Equilibrium statistical mechanics and thermodynamics Statistical dynamics in rotationally inelastic gas-surface scattering: dynamical Lie	
algebraic method, Y. Zheng, X. Yi, D. Guan and Q. Meng	255 (2000) 273
Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S.	255 (2000) 275
Klokishner, J. Linares and F. Varret	255 (2000) 317
A new intermolecular potential energy surface for carbon dioxide from ab initio	()
calculations, S. Bock, E. Bich and E. Vogel	257 (2000) 147
Solvent effect on Sr ²⁺ to Ca ²⁺ ion mutation: Monte Carlo simulation study, HS. Kim	257 (2000) 183
Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes	258 (2000) 201
Extent of inter-hydrogen bond correlations in water. Temperature effect, A. Luzar	258 (2000) 267
On the origin of the heat capacity feature of annealed ices and ice clathrates, and	
interpreting water's diffusivity in terms of the entropy, G.P. Johari	258 (2000) 277
New perspectives on hydrophobic effects, G. Hummer, S. Garde, A.E. García and L.R.	
Pratt	258 (2000) 349
Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin	250 (2000) 405
inhibitor, G.C. Lynch and B.M. Pettitt	258 (2000) 405
Hydration structure of the α-chymotrypsin substrate binding pocket: the impact of constrained geometry, C. Carey, YK. Cheng and P.J. Rossky	259 (2000) 415
Nature of collagen-water hydration forces: a problem in water structure, G.E.	258 (2000) 415
Walrafen and YC. Chu	258 (2000) 427
A rigorous procedure for combining molecular dynamics and Monte Carlo simulation	230 (2000) 427
algorithms, L.J. LaBerge and J.C. Tully	260 (2000) 183
A modified perturbed hard-sphere-chain equation of state: consideration of attractive	, , , , ,
contribution, I.H. Kim and Y.C. Bae	260 (2000) 337
Extramum mathods for ansambles (anaray autrony free anaray)	
Extremum methods for ensembles (energy, entropy, free energy) Monte Carlo simulation study of solvent effect on Na ⁺ to Li ⁺ ion mutation, HS. Kim	253 (2000) 305
With the Carlo simulation study of solvent effect on Na to El Toli mutation, 115. Kim	255 (2000) 505
Time and space correlation functions	
Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and	
M.F. Gelin	252 (2000) 323
Semiclassical description of purely rotational recurrences for collisionless asymmetric	255 (2000) 111
top molecules: new results, M.F. Gelin, V.A. Tolkachev and A.P. Blokhin	255 (2000) 111
Spectral density of medium strength H-bonds. Direct damping and intrinsic	
anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau	256 (2000) 95
The isotopic and temperature dependent properties of hydrogen chloride dissolved in	256 (2000) 85
carbon tetrachloride. A molecular dynamics approach, G. Chatzis and J. Samios	257 (2000) 51
Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G.	237 (2000) 31
Kusalik	258 (2000) 181
Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T.	
Hynes	258 (2000) 201

Experiment

Magnetic resonances		
Calculation of CIDNP field dependences in biradicals in the photolysis of large-ring		
cycloalkanones, A.V. Popov, P.A. Purtov and A.V. Yurkovskaya	252 (2000) 8:	3
Motional effects on optimum coherence transfer in ² H MAS NMR spectroscopy, J.H. Kristensen, G.L. Hoatson and R.L. Vold	252 (2000) 0	7
Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M.	252 (2000) 9	1
Maggini, M. Prato, I. Lamparth and A. Hirsch Q-Band single-crystal EPR study and molecular orbital calculations of [(C ₆ H ₅) ₄ As]- [Re ^{VI} NCl ₄ /Re ^V OCl ₄], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and	253 (2000) 10	15
R. Kirmse	253 (2000) 17	1
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S. Karabunarliev and M. Baumgarten	254 (2000) 23	39
Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W.		
Dwyer	256 (2000) 3	17
Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli	256 (2000) 26	55
Molecular spectroscopy		
Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of the transitions probability from metastable states, B.F. Minaev	252 (2000) 2	25
Temperature-independent onset of diffusion control during polymerization in a diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A.	252 (2000) 2	.5
Wasylyshyn and G.P. Johari	252 (2000) 23	37
Reassignment of ground and first excited state vibrations in phenol, W. Roth, P. Imhof, M. Gerhards, S. Schumm and K. Kleinermanns	252 (2000) 24	1 7
Dielectric relaxation and molecular conformational energy of some arylazo benzothia- zine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and		
A. Jurlewicz	252 (2000) 28	39
Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal	253 (2000) 11	15
Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems:		
ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp The collisional removal of the carbene $CCl_2(\widetilde{X}(0,0,0))$ and $CCl_2(\widetilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	253 (2000) 31	13
Rayo, D. Husain and F. Castaño	254 (2000) 7	77
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup		
and J. Waluk	254 (2000) 13	35
Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G. Baranović	254 (2000) 15	51
Some remarks on the application of relaxation techniques to chemical equilibria, M. Galán and G. Angulo	254 (2000) 32	29

Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S. Santini and R.S. Cataliotti	254 (2000) 337
Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal	254 (2000) 349
Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau	256 (2000) 85
Light intensity dependence of a two-photon catalytic cycle: photoionization via absorption-electron transfer-absorption, M. Goez and V. Zubarev	256 (2000) 107
Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre	, ,
and I. Billard	256 (2000) 307
Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J.W. Rich Laser flash photolysis of IrCl ₆ ²⁻ in aqueous solutions, E.M. Glebov, V.F. Plyusnin, N.V.	256 (2000) 315
Tkachenko and H. Lemmetyinen The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1	257 (2000) 79
state of Cd-Ar, G.D. Roston and M.S. Helmi Semi-empirical study of chain conformation and absorption spectra of polyanilines:	258 (2000) 55
size, solvent and disorder effects, Z.T. de Oliveira and M.C. dos Santos The effect of carbonyl complexation on highly exothermic vanadium oxidation	260 (2000) 95
reactions, M.J. McQuaid and J.L. Gole	260 (2000) 367
-microwave	
DFT and HF-DFT calculations of ¹⁴ N quadrupole coupling constants in molecules, W.C. Bailey	252 (2000) 57
Density functional theory and Hartree–Fock-density functional theory calculations of ¹⁷ O, ³³ S, and ⁷³ Ge quadrupole coupling constants, W.C. Bailey, F.M. Gonzalez and J. Castiglione	260 (2000) 227
3. Castignone	260 (2000) 327
-infrared	
Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study, A. Kovács, G. Keresztury and V. Izvekov	253 (2000) 193
Activation of CO ₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin	254 (2000) 231
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron Photomobility of O(¹ D) atom in solid Ar and its reaction with CF ₃ I, M. Chen, X.	254 (2000) 267
Wang, L. Zhang, Q. Qin and Q. Zheng	255 (2000) 95
Methylation effects on the collisional quenching of vibrationally excited benzene derivatives by unexcited parent molecules, S.Y. Bae, IJ. Lee and J. Park	255 (2000) 103
Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews	255 (2000) 205
Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and	
O. Henri-Rousseau	256 (2000) 85

*	
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E.	
Alikhani and J.P. Perchard Time-resolved Fourier transform infrared spectroscopy of optically pumped	256 (2000) 195
carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and	
J.W. Rich Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y.	256 (2000) 315
Gauduel and H. Gelabert	256 (2000) 333
Analysis of torsion-rotational transitions in the first three torsional states of CH ₃ OD, I. Mukhopadhyay and YB. Duan	257 (2000) 91
High resolution near infrared spectrum of solid nitrogen, pure and doped with carbon	
dioxide, F. Legay and N. Legay-Sommaire Infrared spectra of BeNO and MgNO in solid argon, G.P. Kushto, F. Ding, B. Liang,	257 (2000) 103
X. Wang, A. Citra and L. Andrews	257 (2000) 223
Reorientational motion and hydrogen-bond stretching dynamics in liquid water, H.J.	259 (2000) 222
Bakker, S. Woutersen and HK. Nienhuys The role of water in B-DNAs B _I to B _{II} conformer substates interconversion: a combined study by calorimetry, FT-IR spectroscopy and computer simulation, A. Pichler, S.	258 (2000) 233
Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer An extended SU(2) model for coupled Morse oscillators, M. Carvajal, R. Lemus, A.	258 (2000) 391
Frank, C. Jung and E. Ziemniak	260 (2000) 105
Impulsive IR-multiphoton dissociation of acrolein: observation of non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR fluorescence	
spectroscopy, P.K. Chowdhury	260 (2000) 151
Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the ground state and vibrational analysis, H. Okamoto, H. Inishi, Y. Nakamura, S.	
Kohtani and R. Nakagaki	260 (2000) 193
Vibrational energy storage in high pressure mixtures of diatomic molecules, E. Plönjes, P. Palm, W. Lee, M. D. Chidley, I.V. Adamovich, W. R. Lempert and J.W. Rich	260 (2000) 353
-Raman	
Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman	252 (2000) 102
and computational study, A. Kovács, G. Keresztury and V. Izvekov Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted	253 (2000) 193
geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas	253 (2000) 323
Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa,	
C. Abematsu, S. Yajima and K. Ishii	253 (2000) 331
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino	256 (2000) 117
High resolution study of 1388 cm ⁻¹ CO ₂ vibration by time-domain CARS: spectral exchange and Dicke effect, D.S. Kuznetsov, V.B. Morozov, A.N. Olenin and V.G.	256 (2000) 117
Tunkin	257 (2000) 117
Nature of collagen-water hydration forces: a problem in water structure, G.E.	250 (2000) 15-
Walrafen and YC. Chu Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the	258 (2000) 427
ground state and vibrational analysis, H. Okamoto, H. Inishi, Y. Nakamura, S.	
Kohtani and R. Nakagaki	260 (2000) 193

Vibrational energy storage in high pressure mixtures of diatomic molecules, E. Plönjes, P. Palm, W. Lee, M. D. Chidley, I.V. Adamovich, W. R. Lempert and J.W. Rich	260 (2000) 353
-UV	
Quantitative studies of the photoabsorption of carbonyl sulphide in the valence-shell, S 2p, 2s and C 1s inner-shell regions (4-360 eV) by dipole electron impact spectroscopies, R. Feng, G. Cooper and C.E. Brion An improved calculation method on optical second-order susceptibilities of organic	252 (2000) 359
materials, XL. Zhu, XZ. You, Y. Zhong, Z. Yu and SL. Guo Relaxation of individual rotational levels of the \widetilde{A}^1A_u electronic state of acetylene excited to the $2v_3'$ and $(v_1' + v_3' + v_6')$ vibrational modes, V.I. Makarov and E.	253 (2000) 241
Quiñones Photophysical properties of tris-acetylpyrene derivative of a cryptand in different environments, P. Bandyopadhyay, P.K. Bharadwaj, M. Basu Roy, R. Dutta and S.	253 (2000) 259
Ghosh	255 (2000) 325
Solvent dependence of the intersystem crossing kinetics of thioxanthone, C. Ley, F. Morlet-Savary, P. Jacques and J.P. Fouassier Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for	255 (2000) 335
organic light-emitting diodes, W. Stampor	256 (2000) 351
Vibronic analyses of the lowest singlet-singlet and singlet-triplet band systems of pyridazine, G. Fischer and P. Wormell	257 (2000) 1
Calculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of configuration interaction methods, S. Lacombe, M. Loudet,	
A. Dargelos and J.M. Camou	258 (2000) 1
Twin states and conical intersections in linear polyenes, W. Fuß, Y. Haas and S. Zilberg Temperature dependent photoabsorption cross sections of allene and methylacetylene in the VUV–UV region, F.Z. Chen, D.L. Judge and C.Y.R. Wu	259 (2000) 273
Photoionization studies of C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D.	260 (2000) 215
Scott, F.H. Watson and G.L. Findley The photoabsorption and constant ionic state spectroscopy of vinylbromide, A. Hoxha,	260 (2000) 225
R. Locht, B. Leyh, D. Dehareng, K. Hottmann, H.W. Jochims and H. Baumgrtel	260 (2000) 237
-visible	
Singlet-singlet excited-state absorption and triplet-triplet absorption of <i>meso</i> -tetra- phenylporphine, H. Gratz and A. Penzkofer Photophysical properties of tris-acetylpyrene derivative of a cryptand in different	254 (2000) 363
environments, P. Bandyopadhyay, P.K. Bharadwaj, M. Basu Roy, R. Dutta and S. Ghosh	255 (2000) 325
Solvent dependence of the intersystem crossing kinetics of thioxanthone, C. Ley, F. Morlet-Savary, P. Jacques and J.P. Fouassier	255 (2000) 335
Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclote-tradecane)chromium(III) nitrate, JH. Choi	256 (2000) 29
Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stampor The lowest energy Frenkel and charge-transfer excitons in quasi-one-dimensional	256 (2000) 351
structures: application to MePTCDI and PTCDA crystals, M. Hoffmann, K. Schmidt, T. Fritz, T. Hasche, V.M. Agranovich and K. Leo	258 (2000) 73

	51
The effect of carbonyl complexation on highly exothermic vanadium oxidation reactions, M.J. McQuaid and J.L. Gole	260 (2000) 367
Photon counting and phase fluorimetry	
Excited-state intramolecular proton transfer followed by <i>cis-trans</i> isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka	252 (2000) 01
Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal	253 (2000) 91 253 (2000) 115
Quantum beats in recombination of spin-correlated radical ion pairs with equivalent protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N. Molin	255 (2000) 237
Pressure quenching of positronium in solid biphenyl, T. Goworek, T. Suzuki, E. Hamada, K. Kondo and Y. Ito	
Eigenvalue spectrum of the survival probability of excitation in nonradiative energy transport, E.N. Bodunov, M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G.	255 (2000) 347
Martinho	259 (2000) 49
Effect of solvent polarizability on dual fluorescence of <i>EE</i> -1-phenyl,4-(1'-pyrenyl)-1,3-butadiene, E. Marri, G. Galiazzo, U. Mazzucato and A. Spalletti	260 (2000) 383
Photoelectron and Auger spectroscopy	
The role of Auger decay in hot electron excitation in copper, H. Petek, H. Nagano, M.J.	
Weida and S. Ogawa	251 (2000) 71
Femtosecond electron dynamics at the benzene/Ag(111) interface, K.J. Gaffney, C.M. Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris	251 (2000) 99
Femtosecond two-photon photoemission studies of image-potential states, T. Fauster, C. Reuß, I.L. Shumay and M. Weinelt	251 (2000) 111
Influence of Xe adlayer morphology and electronic structure on image-potential state lifetimes of Ru(0001), W. Berthold, U. Höfer, P. Feulner and D. Menzel	251 (2000) 123
Photoemission linewidths narrower than the quasiparticle inverse lifetime, TC. Chiang Ultrafast electron dynamics at surfaces probed by resonant Auger spectroscopy, W.	251 (2000) 133
Wurth and D. Menzel Quasi-particle lifetimes on noble metal surfaces studied by ARPES and STM, R.	251 (2000) 141
Matzdorf An experimental and theoretical study of the valence shell photoelectron spectrum of bromobenzene, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K.	251 (2000) 151
Siegbahn, A.W. Potts and W. von Niessen Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and	252 (2000) 257
S. Matsuzaki	253 (2000) 125
A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen	253 (2000) 133
A study of the molecular structure and spectroscopic properties of benzo- and pyrido- tetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell	254 (2000) 375
An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	234 (2000) 313
Niessen	254 (2000) 385

Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic \tilde{B} state, A. Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H. Baumgärtel Calculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of configuration interaction methods, S. Lacombe, M. Loudet, A. Dargelos and J.M. Camou An experimental and theoretical study of the HNCO ⁺ ion, S. Wilsey, S.E. Thomas and J.H.D. Eland State selected reactions of krypton ions with methane, A. Kok, P.A.Z. van Emmichoven and A. Niehaus On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, O. Plashkevych, T. Privalov, H. Ågren, V. Carravetta and K. Ruud	256 (2000) 239 258 (2000) 1 258 (2000) 21 258 (2000) 47 260 (2000) 11
Multiphoton ionization Supersonic jet and solution studies of intramolecular complexes with TICT formation	
mimicking solute–solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-	254 (2000) 407
methylcyclopentanone, D. Kim and T. Baer Liquid water ionization: mechanistic implications of the H/D isotope effect in the	256 (2000) 251
geminate recombination of hydrated electrons, M.U. Sander, M.S. Gudiksen, K. Luther and J. Troe Conical intersections, pseudorotation and coherent oscillations in ultrafast photo-	258 (2000) 257
dissociation of group-6 metal hexacarbonyls, S.A. Trushin, W. Fuß and W.E. Schmid	259 (2000) 313
Structure and ground and first electronic excited state vibrational modes of the ethyl-p-aminobenzoate conformers, A. Longarte, J.A. Fernández, I. Unamuno and F.	260 (2000) 02
Castaño The effect of carbonyl complexation on highly exothermic vanadium oxidation reactions, M.J. McQuaid and J.L. Gole	260 (2000) 83 260 (2000) 367
	200 (2000) 307
X-ray spectroscopy The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,	
J. Kawai, M. Takahashi, AM. Vlaicu, H. Adachi and T. Mukoyama A comparison of the oxygen 1s photoabsorption spectra of SO ₂ and NO ₂ , A. Jürgensen	253 (2000) 27
and R.G. Cavell	257 (2000) 123
On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, O. Plashkevych, T. Privalov, H. Ågren, V. Carravetta and K. Ruud	260 (2000) 11
Electron impact spectroscopy	
Quantitative studies of the photoabsorption of carbonyl sulphide in the valence-shell, S 2p, 2s and C 1s inner-shell regions (4–360 eV) by dipole electron impact	
spectroscopies, R. Feng, G. Cooper and C.E. Brion Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V.	252 (2000) 359
Litvinyuk, Y. Zheng and C.E. Brion	253 (2000) 41

Kinetic energy distributions for O ⁻ and metastable CO [*] produced by electron stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y.L. Coat, P.	254 (2000) 60
Cloutier and L. Sanche	254 (2000) 69
Dipole (e,e+ion) coincidence studies of the ionic photofragmentation and photoionization of carbonyl sulfide in the valence shell and S 2p, 2s and C 1s inner shell regions (10–300 eV), R. Feng, G. Cooper, Y. Sakai and C.E. Brion	255 (2000) 353
Generalized oscillator strengths for inner-shell excitation of SF ₆ recorded with a high- performance electron energy loss spectrometer, I.G. Eustatiu, J.T. Francis, T. Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P. Hitchcock	257 (2000) 235
Orbital imaging for the valence shell of sulphur dioxide: comparison of EMS measurements with near Hartree-Fock limit and density functional theory, R. Feng,	
Y. Sakai, Y. Zheng, G. Cooper and C.E. Brion	260 (2000) 29
UV, VUV and soft X-ray photoabsorption of dimethyl ether by dipole (e,e) spectroscopies, R. Feng, G. Cooper and C.E. Brion	260 (2000) 391
Laser induced fluorescence	
Reassignment of ground and first excited state vibrations in phenol, W. Roth, P. Imhof, M. Gerhards, S. Schumm and K. Kleinermanns	252 (2000) 247
Magnetic fluorescence quenching of the NO β(0–9) transition, V.I. Makarov, I.V. Khmelinskii, S.A. Kochubei and V.N. Ishchenko	252 (2000) 379
The collisional removal of the carbene $CCl_2(\widetilde{X}(0,0,0))$ and $CCl_2(\widetilde{A}^{\dagger}B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	
Rayo, D. Husain and F. Castaño	254 (2000) 77
Optical transitions from the chlorine $O_u^+(^3P_2)$ ion-pair state, N.K. Bibinov, A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D.	
Spangenberg and A. Westphal	254 (2000) 349
Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	
and B. Brutschy	254 (2000) 407
Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A.	256 (2000) 125
Costela, I. García-Moreno, R. Sastre and F.J. Duarte Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the distance estimation between trap sites, SG. Kang, WS. Chae, YR. Kim, JS.	256 (2000) 125
Jung and SH. Lee	256 (2000) 295
The anomalous Stark effect of single terrylene molecules in <i>p</i> -terphenyl crystals, P.	250 (2000) 250
Bordat, M. Orrit, R. Brown and A. Würger	258 (2000) 63
Production processes of H(D) atoms in the reactions of NO($A^2\Sigma^+$) with C_2H_2 , C_2H_4 ,	
H ₂ O, and their isotopic variants, H. Umemoto, N. Terada, K. Tanaka, T.	
Takayanagi, Y. Kurosaki and K. Yokoyama	259 (2000) 39
Determination of single-site absorption spectrum in dye-doped disordered materials by double site-selective spectroscopy, Y. Ichino, Y. Kanematsu, A. Kurita and T.	
Kushida	259 (2000) 63
Electronic spectroscopy and structures of the van der Waals complexes of α,ω-	260 (2000) 240
dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer	260 (2000) 249

Linear and convolution methods for the analysis of ground and excited state kinetics. Application to the monomer–excimer scheme, M.N. Berberan-Santos, J.P.S. Farinha	
and J.M.G. Martinho	260 (2000) 401
Relaxation of photo-excitations in films of oligo- and poly-(para-phenylene	
vinylene) derivatives, S.C.J. Meskers, R.A.J. Janssen, J.E.M. Haverkort and	
J.H. Wolter	260 (2000) 415
Ultrafast measurements	
Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanopar-	
ticles, T.V. Shahbazyan and I.E. Perakis	251 (2000) 37
Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in	
desorption, J.W. Gadzuk	251 (2000) 87
Femtosecond electron dynamics at the benzene/Ag(111) interface, K.J. Gaffney, C.M. Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris	251 (2000) 99
Femtosecond two-photon photoemission studies of image-potential states, T. Fauster,	231 (2000) 77
C. Reuß, I.L. Shumay and M. Weinelt	251 (2000) 111
Influence of Xe adlayer morphology and electronic structure on image-potential state	
lifetimes of Ru(0001), W. Berthold, U. Höfer, P. Feulner and D. Menzel	251 (2000) 123
Ultrafast electron and lattice dynamics in semiconductors at high excited carrier densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur	251 (2000) 167
Electron dynamics in metallic nanoparticles, JY. Bigot, V. Halté, JC. Merle and A.	231 (2000) 107
Daunois	251 (2000) 181
Ultrafast transient grating scattering studies of carrier dynamics at a silicon surface, T.	
Sjodin, CM. Li, H. Petek and HL. Dai	251 (2000) 205
Electron dynamics and surface plasmon resonance nonlinearities in metal nanoparti- cles, N. Del Fatti, F. Vallée, C. Flytzanis, Y. Hamanaka and A. Nakamura	251 (2000) 215
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J.	251 (2000) 215
Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell	251 (2000) 227
Electron and lattice dynamics following optical excitation of metals, J. Hohlfeld, SS.	,
Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias	251 (2000) 237
Ultrafast optical relaxation dynamics in metallic nanoparticles: from bulk-like toward	
spatial confinement regime, S. Stagira, M. Nisoli, S. De Silvestri, A. Stella, P. Tognini, P. Cheyssac and R. Kofman	251 (2000) 259
Coherent control of electron–phonon quantum kinetics: exploring the weak and the	231 (2000) 237
strong coupling regime, M. Wegener and D.S. Chemla	251 (2000) 269
Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic	
generation, YM. Chang, L. Xu and H.W.K. Tom Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and	251 (2000) 283
M.F. Gelin	252 (2000) 323
Observation of a bottleneck in the vibrational relaxation of liquid bromoform,	232 (2000) 323
M.A.F.H. van den Broek and H.J. Bakker	253 (2000) 157
Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga,	
M.C. Marconi, R. Martín Negri and P.F. Aramendía	253 (2000) 249
Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W.	
Rettig	253 (2000) 339
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	(
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319

)1

Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra-	
phenylporphine, H. Gratz and A. Penzkofer Solvent dependence of the intersystem crossing kinetics of thioxanthone, C. Ley, F.	254 (2000) 363
Morlet-Savary, P. Jacques and J.P. Fouassier Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P.	255 (2000) 335
Plaza, W. Rettig and M.M. Martin Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y.	256 (2000) 137
Gauduel and H. Gelabert Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H.	256 (2000) 333
Matsui and M. Takeshima	258 (2000) 97
Energy dissipation and relaxation processes in deoxy myoglobin after photoexcitation in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochstrasser Twin states and conical intersections in linear polyenes, W. Fuß, Y. Haas and	259 (2000) 71
S. Zilberg	259 (2000) 273
Dihydroazulene/vinylheptafulvene photochromism: dynamics of the photochemical ring-opening reaction, J. Ern, M. Petermann, T. Mrozek, J. Daub, K. Kuldová and	
C. Kryschi	259 (2000) 331
Nonlinear optics and spectroscopy	
Ultrafast transient grating scattering studies of carrier dynamics at a silicon surface, T. Sjodin, CM. Li, H. Petek and HL. Dai	251 (2000) 205
Electron dynamics and surface plasmon resonance nonlinearities in metal nanoparticles, N. Del Fatti, F. Vallée, C. Flytzanis, Y. Hamanaka and A. Nakamura	251 (2000) 215
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.L Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell	251 (2000) 227
Electron and lattice dynamics following optical excitation of metals, J. Hohlfeld, SS. Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias	251 (2000) 237
Ultrafast optical relaxation dynamics in metallic nanoparticles: from bulk-like toward spatial confinement regime, S. Stagira, M. Nisoli, S. De Silvestri, A. Stella, P.	
Tognini, P. Cheyssac and R. Kofman Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic	251 (2000) 259
generation, YM. Chang, L. Xu and H.W.K. Tom Zwitterionic polymers for nonlinear optics, C. Combellas, F. Kajzar, G. Mathey, M.A.	251 (2000) 283
Petit and A. Thiébault Singlet-singlet excited-state absorption and triplet-triplet absorption of <i>meso</i> -tetra-	252 (2000) 165
phenylporphine, H. Gratz and A. Penzkofer Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate	254 (2000) 363
methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte	256 (2000) 125
Optical spectroscopy and crystal-field effects on the paramagnetic susceptibility of rare-earth germanates $GaRGe_2O_7$, $R=Pr$, Nd, C. Cascales, G. Lozano, C. Zaldo and P.	230 (2000) 123
Porcher	257 (2000) 29
Electroabsorption spectroscopy of distyrylbenzene derivatives, P.A. Lane, H. Mellor, S.J. Martin, T.W. Hagler, A. Bleyer and D.D.C. Bradley	257 (2000) 41
High resolution study of 1388 cm ⁻¹ CO ₂ vibration by time-domain CARS: spectral exchange and Dicke effect, D.S. Kuznetsov, V.B. Morozov, A.N. Olenin and V.G.	
Tunkin	257 (2000) 117

Dispersive photoelectron spectroscopy of the ungerade Rydberg states of Xe ₂ near Xe*(6p,5d), D.M. Mao, X.K. Hu, Y.J. Shi and R.H. Lipson Optimization of the molecular hyperpolarizability for second harmonic generation in	257 (2000) 253
chiral media, V. Ostroverkhov, O. Ostroverkhova, R.G. Petschek, K.D. Singer, L. Sukhomlinova, R.J. Twieg, SX. Wang and L.C. Chien Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W.	257 (2000) 263
Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis A theoretical analysis of the sum frequency generation spectrum of the water surface, A.	257 (2000) 275
Morita and J.T. Hynes Relaxation processes in singlet O ₂ analyzed by laser-induced gratings, W. Hubschmid	258 (2000) 371
and B. Hemmerling	259 (2000) 109
Vibrational corrections to linear and nonlinear static electric properties of polyatomic molecules at non-optimum reference geometry, V.E. Ingamells, M.G. Papadopoulos	
and A.J. Sadlej	260 (2000) 1
Synchrotron spectroscopies	251 (2000) 122
Photoemission linewidths narrower than the quasiparticle inverse lifetime, TC. Chiang Ultrafast electron dynamics at surfaces probed by resonant Auger spectroscopy, W.	251 (2000) 133
Wurth and D. Menzel An experimental and theoretical study of the valence shell photoelectron spectrum of	251 (2000) 141
bromobenzene, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen	252 (2000) 257
A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson,	
R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen Energy dependences of fragment ion yields from acetone photoexcited in the C1s and	253 (2000) 133
Ols transition regions, I.H. Suzuki and N. Saito An experimental and theoretical study of the valence shell photoelectron spectrum of	253 (2000) 351
the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	
Niessen Photodissociation spectroscopy of CICN in the vacuum ultraviolet region, K. Kanda,	254 (2000) 385
M. Kono, T. Nagata, A. Hiraya, K. Tabayashi and K. Shobatake About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine	255 (2000) 369
structure and its vibrational analysis, R. Locht, B. Leyh, A. Hoxha, D. Dehareng,	257 (2000) 202
H.W. Jochims and H. Baumgärtel Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV photon	257 (2000) 283
energy range, M. Schwell, F. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H. Baumgrtel and S. Leach	260 (2000) 261
Coherent optical spectroscopy	
Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shahbazyan and I.E. Perakis	251 (2000) 37
Coherent control of electron-phonon quantum kinetics: exploring the weak and the strong coupling regime, M. Wegener and D.S. Chemla	251 (2000) 269
Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic generation, YM. Chang, L. Xu and H.W.K. Tom	251 (2000) 283
generation, 1W. Chang, L. Au and H. W.K. Tom	231 (2000) 283

)9

21
251 (2000) 309
254 (2000) 25
256 (2000) 315
252 (2000) 247
255 (2000) 379
254 (2000) 169
252 (2000) 179
252 (2000) 250
253 (2000) 259
255 (2000) 273
256 (2000) 259
258 (2000) 291
250 (2000) 271
260 (2000) 143
253 (2000) 59
255 (2000) 57
253 (2000) 351
254 (2000) 69
258 (2000) 13
258 (2000) 21

State selected reactions of krypton ions with methane, A. Kok, P.A.Z. van	
Emmichoven and A. Niehaus Structure and ground and first electronic excited state vibrational modes of the ethyl-p-	258 (2000) 47
aminobenzoate conformers, A. Longarte, J.A. Fernández, Iñ. Unamuno and F. Castaño	260 (2000) 83
Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV photon energy range, M. Schwell, F.v. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H.	240 (2000) 241
Baumgrtel and S. Leach Vertical triple ionization of ethyne molecules in triple-electron-transfer collisions with	260 (2000) 261
O ²⁺ beam ions, N. Jeffreys, D.E. Parry and F.M. Harris	260 (2000) 295
Radiolysis	
Influence of geminate recombination kinetics on the shape of low field MARY line,	
Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin	253 (2000) 231
X-ray, electron and neutron diffraction	
The radial distribution functions of water and ice from 220 to 673 K and at pressures up	259 (2000) 121
to 400 MPa, A.K. Soper Anomalous X-ray diffraction studies of hydration effects in concentrated aqueous	258 (2000) 121
electrolyte solutions, S. Ramos, A.C. Barnes, G.W. Neilson and M.J. Capitan	258 (2000) 171
Neutron scattering (inelastic and quasielastic)	
The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and	
J.M. Simonson	258 (2000) 109
Generalized frequency spectra of water at both sides of the freezing transition, J. Dawidowski, F.J. Bermejo, C. Cabrillo and S.M. Bennington	258 (2000) 247
Extent of inter-hydrogen bond correlations in water. Temperature effect, A. Luzar	258 (2000) 267
Relaxational dynamics of water molecules at protein surface, S. Dellerue and MC.	
Bellissent-Funel	258 (2000) 315
Small angle X-ray and neutron diffraction	
Structural studies of water in confined geometry by neutron diffraction, J. Dore	258 (2000) 327
Light scattering	
Mandelstam-Brillouin spectra and hyperacoustic velocities dispersion of trideuteroa-	255 (2000) 05
cetonitrile in the liquid state, R.S. Cataliotti, P. Sassi, A. Morresi and G. Paliani First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J.	255 (2000) 85
Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
Scanning tunneling and force microscopies	
Quasi-particle lifetimes on noble metal surfaces studied by ARPES and STM, R.	
Matzdorf	251 (2000) 151

252 (2000) 115

253 (2000) 205

253 (2000) 259

254 (2000) 77

Calorimetric methods	
Dielectric relaxations of collagen and elastin in the dehydrated state, V. Samouillan, A.	
Lamure and C. Lacabanne	255 (2000) 259
On the origin of the heat capacity feature of annealed ices and ice clathrates, and	, , , , , , , , , , , , , , , , , , , ,
interpreting water's diffusivity in terms of the entropy, G.P. Johari	258 (2000) 277
The role of water in B-DNAs B ₁ to B ₁₁ conformer substates interconversion: a combined	
study by calorimetry, FT-IR spectroscopy and computer simulation, A. Pichler, S.	
Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer	258 (2000) 391
Measurement of macroscopic variables	
Self-diffusion in liquid metals, A.S. Chauhan, R. Ravi and R.P. Chhabra	252 (2000) 227
Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E.	
Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri	253 (2000) 205
Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-	
nitro)- and 1-(3-aminophenyl)-1H-methanofullerene doped with cobaltocene, P.	
Umek, A. Omerzu, D. Mihailović and M. Tokumoto	253 (2000) 361
Some remarks on the application of relaxation techniques to chemical equilibria, M.	
Galán and G. Angulo	254 (2000) 329

Objects

5

1

15

85

89

51

Bulk systems

Gases
The attractive quartet potential energy surface for the CH ₃ C(a ⁴ A ₂) + CO ₁
Hou B Wang and Y Gu

reaction, H. 252 (2000) 17

Electron-photon field dynamics: numerically exact calculations of multi-state molecule systems interacting with a single-mode coherent photon field, M. Nakano and K. Yamaguchi

Time-dependent quantum dynamics study of reactive scattering of the HD + CN system in the potential averaged 5D model, Y. Zhang, Z. Tan, H. Zhang, Q. Zhang and J.Z.H. Zhang 252 (2000) 191

The electron localization function description of aromaticity in five-membered rings, D.B. Chesnut and L.J. Bartolotti 253 (2000) 1

Protonation of archetypal aromatic and antiaromatic systems - G2 studies of benzene and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59

Kinetics of the reactions of FC(O)O₂ radicals with F atoms and F₂, M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri

Relaxation of individual rotational levels of the A Au electronic state of acetylene excited to the $2v_3$ and $(v_1' + v_3' + v_6')$ vibrational modes, V.I. Makarov and E.

Quiñones The collisional removal of the carbene $CCl_2(X(0,0,0))$ and $CCl_2(A^{\dagger}B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño

Optical transitions from the chlorine $O_u^+(^3P_2)$ ion-pair state, N.K. Bibinov, A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
Ground and excited states of isodiazene - an ab initio study, V. Stepanić and G.	
Baranović Structural properties and quantum effects in protonated helium clusters. I. The ab initio	254 (2000) 151
interaction potential, B. Balta and F.A. Gianturco	254 (2000) 203
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	254 (2000) 215
Paesani Broadening and shifting coefficients of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure H_2 : coupled states and semiclassical calculations. Comparison with experiments, X .	254 (2000) 215
Bruet, J. Bonamy and M.L. Dubernet-Tuckey Kinetic modelling of radiative reacting gas flow under strong nonequilibrium	254 (2000) 297
conditions, E.V. Kustova and A. Chikhaoui Methylation effects on the collisional quenching of vibrationally excited benzene	255 (2000) 59
derivatives by unexcited parent molecules, S.Y. Bae, IJ. Lee and J. Park Laser-induced amplified spontaneous emission from the 3d and nf Rydberg states of	255 (2000) 103
NO, Y. Ogi, M. Takahashi, K. Tsukiyama and R. Bersohn Reactant-product decoupling approach to state-to-state reactive scattering H+DH, S.	255 (2000) 379
Zhang, Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang Theoretical study of the infrared and ultraviolet spectrum of the radical F ₂ CN, H.	255 (2000) 397
Dupin, I. Baraille, C. Larrieu and A. Dargelos Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion	256 (2000) 7
chambers, A.L. Itkin Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-	256 (2000) 61
methylcyclopentanone, D. Kim and T. Baer	256 (2000) 251
Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli	256 (2000) 265
Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J.W. Rich	256 (2000) 315
Vibronic analyses of the lowest singlet-singlet and singlet-triplet band systems of pyridazine, G. Fischer and P. Wormell	257 (2000) 1
A proper mobility formula for large, heavy particles in gases in any regime, L. Ferrari High resolution study of 1388 cm ⁻¹ CO ₂ vibration by time-domain CARS: spectral exchange and Dicke effect, D.S. Kuznetsov, V.B. Morozov, A.N. Olenin and V.G.	257 (2000) 63
Tunkin A comparison of the oxygen 1s photoabsorption spectra of SO ₂ and NO ₂ , A. Jürgensen	257 (2000) 117
and R.G. Cavell A new intermolecular potential energy surface for carbon dioxide from ab initio	257 (2000) 123
calculations, S. Bock, E. Bich and E. Vogel Quasi-classical dynamics and vibrational kinetics of $N + N_2(v)$ system, F. Esposito, M.	257 (2000) 147
Capitelli and C. Gorse	257 (2000) 193
Generalized oscillator strengths for inner-shell excitation of SF ₆ recorded with a high- performance electron energy loss spectrometer, I.G. Eustatiu, J.T. Francis, T. Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P. Hitchcock	257 (2000) 235
About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine structure and its vibrational analysis, R. Locht, B. Leyh, A. Hoxha, D. Dehareng, H.W. Jochims and H. Baumgärtel	257 (2000) 283
	20. (2000) 200

Calculation of the electronic and photoelectronic spectra of nitroso compounds: a reinvestigation by use of configuration interaction methods, S. Lacombe, M. Loudet,		
A. Dargelos and J.M. Camou Mass spectra and theoretical modeling of Li^+Ne_n , Li^+Ar_n and Li^+Kr_n clusters, G.E.	258 (2000)	1
Froudakis, S.C. Farantos and M. Velegrakis Relaxation processes in singlet O ₂ analyzed by laser-induced gratings, W. Hubschmid	258 (2000)	13
and B. Hemmerling	259 (2000)	109
The geometric phase effect in chemical reactions, S. Adhikari and G.D. Billing Twin states and conical intersections in linear polyenes, W. Fuß, Y. Haas and	259 (2000)	149
S. Zilberg On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, O. Plashkevych, T. Privalov,	259 (2000)	
H. Ågren, V. Carravetta and K. Ruud An extended SU(2) model for coupled Morse oscillators, M. Carvajal, R. Lemus, A.	260 (2000)	
Frank, C. Jung and E. Ziemniak Impulsive IR-multiphoton dissociation of acrolein: observation of non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR fluorescence	260 (2000)	
spectroscopy, P.K. Chowdhury Temperature dependent photoabsorption cross sections of allene and methylacetylene in the VUV-UV region, F.Z. Chen, D.L. Judge and C.Y.R. Wu	260 (2000) 260 (2000)	
Photoionization studies of C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D. Scott, F.H. Watson and G.L. Findley	260 (2000)	
Ab initio calculation for inner reorganization energy of gas-phase electron transfer in organic molecule-ion systems, XY. Li, J. Tong and FC. He	260 (2000)	283
Density functional theory and Hartree–Fock-density functional theory calculations of ¹⁷ O, ³³ S, and ⁷³ Ge quadrupole coupling constants, W.C. Bailey, F.M. Gonzalez and J. Castiglione	260 (2000)	327
Supergonia hagus		
Supersonic beams Reassignment of ground and first excited state vibrations in phenol, W. Roth, P. Imhof,		
M. Gerhards, S. Schumm and K. Kleinermanns The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-	252 (2000)	247
Quraishi Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	252 (2000)	337
and B. Brutschy Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E.	254 (2000)	407
Alikhani and J.P. Perchard Structure and ground and first electronic excited state vibrational modes of the ethyl-paminobenzoate conformers, A. Longarte, J.A. Fernández, Iñ. Unamuno and F.	256 (2000)	195
Castaño	260 (2000)) 83
Liquids neat		
Observation of a bottleneck in the vibrational relaxation of liquid bromoform, M.A.F.H. van den Broek and H.J. Bakker	253 (2000)	157
Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman	253 (2000)	
	,	

Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted	
geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas Mandelstam–Brillouin spectra and hyperacoustic velocities dispersion of trideuteroa-	253 (2000) 323
cetonitrile in the liquid state, R.S. Cataliotti, P. Sassi, A. Morresi and G. Paliani	255 (2000) 85
The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and	
J.M. Simonson	258 (2000) 109
The radial distribution functions of water and ice from 220 to 673 K and at pressures up	
to 400 MPa, A.K. Soper Reorientational motion and hydrogen-bond stretching dynamics in liquid water, H.J.	258 (2000) 121
Bakker, S. Woutersen and HK. Nienhuys	258 (2000) 233
Generalized frequency spectra of water at both sides of the freezing transition, J.	,
Dawidowski, F.J. Bermejo, C. Cabrillo and S.M. Bennington	258 (2000) 247
Liquid water ionization: mechanistic implications of the H/D isotope effect in the geminate recombination of hydrated electrons, M.U. Sander, M.S. Gudiksen, K.	
Luther and J. Troe	258 (2000) 257
Extent of inter-hydrogen bond correlations in water. Temperature effect, A. Luzar	258 (2000) 267
Slow dynamics in supercooled water, F. Sciortino Structural studies of water in confined geometry by neutron diffraction, J. Dore	258 (2000) 307 258 (2000) 327
Structural studies of water in confined geometry by neutron diffraction, J. Dore	238 (2000) 327
Liquid mixtures and solutions	
Calculation of CIDNP field dependences in biradicals in the photolysis of large-ring	
cycloalkanones, A.V. Popov, P.A. Purtov and A.V. Yurkovskaya Temperature-independent onset of diffusion control during polymerization in a	252 (2000) 83
diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A.	252 (2000) 227
Wasylyshyn and G.P. Johari The solvent influence on the electrochemical transfer of divalent ions, O. Pecina and W.	252 (2000) 237
Schmickler	252 (2000) 349
Excited-state intramolecular proton transfer followed by cis-trans isomerization of (1-	
hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka	253 (2000) 91
Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga,	233 (2000) 91
M.C. Marconi, R. Martín Negri and P.F. Aramendía	253 (2000) 249
Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W.	
Rettig	253 (2000) 339
Role of inertial and non-Markovian effects on activated barrier crossing dynamics for charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic	254 (2000) 57
solvents, M.V. Veng, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Some remarks on the application of relaxation techniques to chemical equilibria, M. Galán and G. Angulo	254 (2000) 220
Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes	254 (2000) 329
in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.	
Santini and R.S. Cataliotti	254 (2000) 337
Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón	255 (2000) 73
association in aqueous solution, b. 10105a, A. Hidaigo and J.A. Sanson	233 (2000) 13

Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-dichloropropane in carbon tetrachloride, S. Madurga, J.C. Paniagua and E.	
Vilaseca	255 (2000) 123
Quantum beats in recombination of spin-correlated radical ion pairs with equivalent protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N.	
Molin	255 (2000) 237
Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P.	
Plaza, W. Rettig and M.M. Martin	256 (2000) 137
The isotopic and temperature dependent properties of hydrogen chloride dissolved in carbon tetrachloride. A molecular dynamics approach, G. Chatzis and J.	
Samios	257 (2000) 51
Laser flash photolysis of IrCl ² ₆ in aqueous solutions, E.M. Glebov, V.F. Plyusnin, N.V. Tkachenko and H. Lemmetyinen	257 (2000) 79
	4
Computation of the pK of liquid water using coordination constraints, M. Sprik	258 (2000) 139
A theoretical study on a Diels-Alder reaction in ambient and supercritical water: viewing solvent effects through frontier orbitals, Y. Harano, H. Sato and F.	
Hirata	258 (2000) 151
Structural and dynamical behavior of an azide anion in water from ab initio molecular	
dynamics calculations, D.A. Yarne, M.E. Tuckerman and M.L. Klein	258 (2000) 163
Anomalous X-ray diffraction studies of hydration effects in concentrated aqueous	, , , , , , , , , , , , , , , , , , , ,
electrolyte solutions, S. Ramos, A.C. Barnes, G.W. Neilson and M.J. Capitan A multi-state empirical valence bond model for acid-base chemistry in aqueous	258 (2000) 171
solution, M. uma, U.W. Schmitt and G.A. Voth	258 (2000) 187
New perspectives on hydrophobic effects, G. Hummer, S. Garde, A.E. García and L.R. Pratt	259 (2000) 240
	258 (2000) 349
Eigenvalue spectrum of the survival probability of excitation in nonradiative energy transport, E.N. Bodunov, M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G.	
Martinho	259 (2000) 49
Twin states and conical intersections in linear polyenes, W. Fuß, Y. Haas and	
S. Zilberg	259 (2000) 273
Dihydroazulene/vinylheptafulvene photochromism: dynamics of the photochemical ring-opening reaction, J. Ern, M. Petermann, T. Mrozek, J. Daub, K. Kuldová and	,,
C. Kryschi	259 (2000) 331
Semi-empirical study of chain conformation and absorption spectra of polyanilines: size, solvent and disorder effects, Z.T. de Oliveira and M.C. dos Santos	
Intermolecular potential for benzoic acid-water based on the test-particle model and	260 (2000) 95
statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	
and B.M. Rode	260 (2000) 159
A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully	260 (2000) 183
Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the ground state and vibrational analysis, H. Okamoto, H. Inishi, Y. Nakamura, S.	
	260 (2000) 102
Kohtani and R. Nakagaki	260 (2000) 193
A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae	260 (2000) 337
Linear and convolution methods for the analysis of ground and excited state kinetics. Application to the monomer–excimer scheme, M.N. Berberan-Santos, J.P.S. Farinha	
and J.M.G. Martinho	260 (2000) 401
	, ,

)9

Crystals		
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M. Pitarke, E.V. Chulkov and A. Rubio	251 (2000)	1
Electronic and structural properties of CaH ₂ : an ab initio Hartree–Fock study, A. El	231 (2000)	
Gridani and M. El Mouhtadi	252 (2000)	1
An improved calculation method on optical second-order susceptibilities of organic materials, XL. Zhu, XZ. You, Y. Zhong, Z. Yu and SL. Guo	253 (2000) 24	41
Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg	253 (2000) 25	
Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	255 (2000) 20	03
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000)	25
A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band theory, XL. Zhu, XZ. You and Y. Zhang Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S.	254 (2000) 28	87
Klokishner, J. Linares and F. Varret	255 (2000) 31	17
Hartree–Fock crystal orbital calculation on sodium-intercalated fullerites C ₆₀ Na ₁₀ and	256 (2000) 1	40
C ₆₀ Na ₁₁ , E.B. Starikov Prediction of pure electric-dipole two-photon absorption circular dichroism in	256 (2000) 14	49
lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the	256 (2000) 20	07
distance estimation between trap sites, SG. Kang, WS. Chae, YR. Kim, JS.		
Jung and SH. Lee Optical spectroscopy and crystal-field effects on the paramagnetic susceptibility of rare-	256 (2000) 29	95
earth germanates GaRGe ₂ O ₇ , R = Pr, Nd, C. Cascales, G. Lozano, C. Zaldo and P.		
Porcher	257 (2000)	29
-neat		
Photoemission linewidths narrower than the quasiparticle inverse lifetime, TC. Chiang An improved calculation method on optical second-order susceptibilities of organic	251 (2000) 1	33
materials, XL. Zhu, XZ. You, Y. Zhong, Z. Yu and SL. Guo	253 (2000) 2	41
Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret	255 (2000) 3	17
Pressure quenching of positronium in solid biphenyl, T. Goworek, T. Suzuki, E.	200 (2000) 5	
Hamada, K. Kondo and Y. Ito Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P.	255 (2000) 3	47
Postorino	256 (2000) 1	17
The lowest energy Frenkel and charge-transfer excitons in quasi-one-dimensional structures: application to MePTCDI and PTCDA crystals, M. Hoffmann, K.	,	
Schmidt, T. Fritz, T. Hasche, V.M. Agranovich and K. Leo On the origin of the heat capacity feature of annealed ices and ice clathrates, and	258 (2000)	73
interpreting water's diffusivity in terms of the entropy, G.P. Johani	258 (2000) 2	277
-mixed		
Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-nitro)- and 1-(3-aminophenyl) ¹ <i>H</i> -methanofullerene doped with cobaltocene, P.		
Umek, A. Omerzu, D. Mihailović and M. Tokumoto	253 (2000) 3	361

)7

Subject index to volumes 251–260	65
Hartree–Fock crystal orbital calculation on sodium-intercalated fullerites $C_{60}Na_{10}$ and $C_{60}Na_{11}$, E.B. Starikov	256 (2000) 149
Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis	257 (2000) 275
The anomalous Stark effect of single terrylene molecules in <i>p</i> -terphenyl crystals, P. Bordat, M. Orrit, R. Brown and A. Würger	258 (2000) 63
Boldat, M. Offit, R. Blown and A. Wulger	238 (2000) 63
Glasses Molecular motions in molecular glasses as studied by thermally stimulated depolarisa-	
tion currents (TSDC), N.T. Correia, C. Alvarez, J.J. Moura Ramos and M.	
Descamps On the origin of the heat capacity feature of annealed ices and ice clathrates, and	252 (2000) 151
interpreting water's diffusivity in terms of the entropy, G.P. Johari The self-diffusivity of amorphous solid water near 150 K, R.S. Smith, Z. Dohnálek,	258 (2000) 277
G.A. Kimmel, K.P. Stevenson and B.D. Kay	258 (2000) 291
The role of water in B-DNAs B _I to B _{II} conformer substates interconversion: a combined study by calorimetry, FT-IR spectroscopy and computer simulation, A. Pichler, S.	
Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer	258 (2000) 391
Complex fluids	
Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	253 (2000) 267
charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik	258 (2000) 181
-liquid crystals	
Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave	
number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii	253 (2000) 331
-micelles	
Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of	252 (2000) 115
the surfactant aerosol-OT, A.K. Mandal and M.K. Pal Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron	253 (2000) 115
annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre and I. Billard	256 (2000) 307
Polymers	
Zwitterionic polymers for nonlinear optics, C. Combellas, F. Kajzar, G. Mathey, M.A. Petit and A. Thiébault	252 (2000) 165
Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	232 (2000) 103
H. Treml and HH. Kohler Temperature-independent onset of diffusion control during polymerization in a	252 (2000) 199
diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A.	
Wasylyshyn and G.P. Johari Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis	252 (2000) 237
and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M.	
Maggini, M. Prato, I. Lamparth and A. Hirsch	253 (2000) 105

*	
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
Magnetic exchange interaction between π-electron radicals adsorbed on graphites, N. Tyutyulkov, F. Dietz and K. Müllen	255 (2000) 223
Influence of the local electric field on ionic transport during redox switching of conducting polymers, F. Miomandre, M.N. Bussac, E. Vieil and L. Zuppiroli	255 (2000) 291
Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A.	,
Costela, I. García-Moreno, R. Sastre and F.J. Duarte Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H.	256 (2000) 125
Matsui and M. Takeshima Determination of single-site absorption spectrum in dye-doped disordered materials by double site-selective spectroscopy, Y. Ichino, Y. Kanematsu, A. Kurita and T.	258 (2000) 97
Kushida	259 (2000) 63
Relaxation of photo-excitations in films of oligo- and poly-(para-phenylene vinylene) derivatives, S.C.J. Meskers, R.A.J. Janssen, J.E.M. Haverkort and J.H. Wolter	260 (2000) 415
Semiconductors	
Ultrafast electron and lattice dynamics in semiconductors at high excited carrier densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur	251 (2000) 167
Ultrafast transient grating scattering studies of carrier dynamics at a silicon surface, T. Sjodin, CM. Li, H. Petek and HL. Dai	251 (2000) 205
Coherent control of electron-phonon quantum kinetics: exploring the weak and the strong coupling regime, M. Wegener and D.S. Chemla	251 (2000) 269
Coherence control of currents in semiconductors: a materials perspective, H.M. van Driel	251 (2000) 309
Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and	
S. Matsuzaki	253 (2000) 125
Metals and alloys	
The role of Auger decay in hot electron excitation in copper, H. Petek, H. Nagano, M.J. Weida and S. Ogawa	251 (2000) 71
Electron dynamics and surface plasmon resonance nonlinearities in metal nanoparticles, N. Del Fatti, F. Vallée, C. Flytzanis, Y. Hamanaka and A. Nakamura	251 (2000) 215
Self-diffusion in liquid metals, A.S. Chauhan, R. Ravi and R.P. Chhabra	251 (2000) 215 252 (2000) 227
Spectral properties and ligand field analysis of cis-dinitrito(1,4,8,11-tetraazacyclote-	,
tradecane)chromium(III) nitrate, JH. Choi	256 (2000) 29
Thin films	
Femtosecond electron dynamics at the benzene/Ag(111) interface, KJ, Gaffney, C.M. Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris	251 (2000) 99
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J.	
Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell	251 (2000) 227

)9

,	
Electron and lattice dynamics following optical excitation of metals, J. Hohlfeld, SS.	
Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias	251 (2000) 237
Zwitterionic polymers for nonlinear optics, C. Combellas, F. Kajzar, G. Mathey, M.A.	
Petit and A. Thiébault	252 (2000) 165
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low	
temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	254 (2000) 240
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319
Infrared spectra of monomeric L-alanine and L-alanine-N-d ₃ zwitterions isolated in a KBr matrix, X. Cao and G. Fischer	255 (2000) 195
Influence of the local electric field on ionic transport during redox switching of	255 (2000) 195
conducting polymers, F. Miomandre, M.N. Bussac, E. Vieil and L. Zuppiroli	255 (2000) 291
Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for	233 (2000) 231
organic light-emitting diodes, W. Stampor	256 (2000) 351
The self-diffusivity of amorphous solid water near 150 K, R.S. Smith, Z. Dohnálek,	()
G.A. Kimmel, K.P. Stevenson and B.D. Kay	258 (2000) 291
Surfaces Theory of indestic lifetimes of law energy electrons in motels DM Echanicus LM	
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M. Pitarke, E.V. Chulkov and A. Rubio	251 (2000) 1
Photodesorption of NO from a metal surface: quantum dynamical implications of a	231 (2000) 1
two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce	251 (2000) 51
Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in	231 (2000) 31
desorption, J.W. Gadzuk	251 (2000) 87
Femtosecond electron dynamics at the benzene/Ag(111) interface, K.J. Gaffney, C.M.	
Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris	251 (2000) 99
Femtosecond two-photon photoemission studies of image-potential states, T. Fauster,	
C. Reuß, I.L. Shumay and M. Weinelt	251 (2000) 111
Influence of Xe adlayer morphology and electronic structure on image-potential state	
lifetimes of Ru(0001), W. Berthold, U. Höfer, P. Feulner and D. Menzel	251 (2000) 123
Quasi-particle lifetimes on noble metal surfaces studied by ARPES and STM, R.	
Matzdorf	251 (2000) 151
Ultrafast transient grating scattering studies of carrier dynamics at a silicon surface, T. Sjodin, CM. Li, H. Petek and HL. Dai	251 (2000) 205
Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic	251 (2000) 205
generation, YM. Chang, L. Xu and H.W.K. Tom	251 (2000) 283
Dynamical Lie algebraic approach to rotationally inelastic scattering of molecules from	231 (2000) 203
surfaces, D. Guan, X. Yi, Y. Zheng, S. Ding and J. Sun	252 (2000) 179
Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted	(
geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas	253 (2000) 323
Kinetic energy distributions for O- and metastable CO* produced by electron	
stimulated desorption from condensed CO2, M. Tronc, R. Azria, Y.L. Coat, P.	
Cloutier and L. Sanche	254 (2000) 69
Order and disorder signatures in the specular scattering intensity of He particles from	
adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco	256 (2000) 259
A theoretical analysis of the sum frequency generation spectrum of the water surface, A.	250 (2000) 251
Morita and J.T. Hynes	258 (2000) 371

Low-dimensional materials Electron dynamics in metallic nanoparticles, JY. Bigot, V. Halté, JC. Merle and A.	
Daunois	251 (2000) 181
Ultrafast optical relaxation dynamics in metallic nanoparticles: from bulk-like toward	201 (2000) 101
spatial confinement regime, S. Stagira, M, Nisoli, S. De Silvestri, A. Stella, P.	
Tognini, P. Cheyssac and R. Kofman	251 (2000) 259
Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret	255 (2000) 317
Klokishner, J. Linares and F. Varret	233 (2000) 317
Dielectrics	
Molecular motions in molecular glasses as studied by thermally stimulated depolarisa-	
tion currents (TSDC), N.T. Correia, C. Alvarez, J.J. Moura Ramos and M.	
Descamps	252 (2000) 151
Temperature-independent onset of diffusion control during polymerization in a diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A.	
Wasylyshyn and G.P. Johari	252 (2000) 237
Dielectric relaxation and molecular conformational energy of some arylazo benzothia-	232 (2000) 231
zine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and A.	
Jurlewicz	252 (2000) 289
DI.	
Plasmas Quasi-classical dynamics and vibrational kinetics of $N + N_2(v)$ system, F. Esposito, M.	
Capitelli and C. Gorse	257 (2000) 193
cupiton and or some	237 (2000) 173
Biological systems	
The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical study	
using combined discrete/self-consistent reaction field models, C. Alemán	253 (2000) 13
Vibronic model of hyperfine interaction in dimeric mixed-valence clusters, A.V. Palii, M.I. Belinsky and B.S. Tsukerblat	255 (2000) 51
Structures, vibrational absorption and vibrational circular dichroism spectra of L-	255 (2000) 51
alanine in aqueous solution: a density functional theory and RHF study, K.	
Frimand, H. Bohr, K.J. Jalkanen and S. Suhai	255 (2000) 165
Energy dissipation and relaxation processes in deoxy myoglobin after photoexcitation	
in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochstrasser	259 (2000) 71
A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully	260 (2000) 183
algorithms, E.J. Laberge and J.C. Tully	200 (2000) 183
Microscopic and mesoscopic systems	
Single atoms, molecules and assemblies (incl. biological)	
Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in	
desorption, J.W. Gadzuk	251 (2000) 87
DFT and HF-DFT calculations of ¹⁴ N quadrupole coupling constants in molecules,	
W.C. Bailey	252 (2000) 57
Electron-photon field dynamics: numerically exact calculations of multi-state molecule	
systems interacting with a single-mode coherent photon field, M. Nakano and K. Yamaguchi	252 (2000) 115
* contrad court	232 (2000) 113

Self-diffusion in liquid metals, A.S. Chauhan, R. Ravi and R.P. Chhabra Photomobility of O(¹ D) atom in solid Ar and its reaction with CF ₃ I, M. Chen, X.	252 (2000) 227
Wang, L. Zhang, Q. Qin and Q. Zheng	255 (2000) 05
Semiclassical description of purely rotational recurrences for collisionless	255 (2000) 95
asymmetric top molecules: new results, M.F. Gelin, V.A. Tolkachev and A.P.	255 (2000) 111
Blokhin	255 (2000) 111
Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-	256 (2000) 251
methylcyclopentanone, D. Kim and T. Baer	256 (2000) 251
A proper mobility formula for large, heavy particles in gases in any regime, L. Ferrari Ab initio study of the $F_2(X^1\Sigma_g^+)$ - $H(^2S)$ van der Waals complex, V. Lukeš, M.	257 (2000) 63
Bittererová, V. Laurinc and S. Biskupič	257 (2000) 157
The pair density description of aromaticity in some substituted cyclopentadienyl systems: a comparison of AIM and ELF bonding descriptors, D.B. Chesnut and L.J.	
Bartolotti	257 (2000) 175
Analysis of the bound odd-parity spectrum of krypton by weakest bound electron	
potential model theory, N.W. Zheng, T. Zhou, R. Yang, T. Wang and D. Ma The anomalous Stark effect of single terrylene molecules in <i>p</i> -terphenyl crystals, P.	258 (2000) 37
Bordat, M. Orrit, R. Brown and A. Würger	258 (2000) 63
A recursive Kohn variational algorithm for the Green's operator: application to the T-	
matrix, D. Brown	259 (2000) 11
Ab initio study of the reaction mechanism of singlet and triplet N ₂ O and their intersystem crossing, DY. Hwang and A.M. Mebel	259 (2000) 89
A model study of the wavepacket dynamics around a Jahn-Teller conical intersection in	
a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani	259 (2000) 201
Density functional theory and Hartree–Fock-density functional theory calculations of ¹⁷ O, ³³ S, and ⁷³ Ge quadrupole coupling constants, W.C. Bailey, F.M. Gonzalez and	
J. Castiglione	260 (2000) 327
Molecules (neutral and ionic)	
Gaussian Type Orbitals basis sets for the calculation of continuum properties in molecules: the differential photoionization cross section of acetylene, I. Cacelli, R.	
Moccia and A. Rizzo	252 (2000) 67
Dielectric relaxation and molecular conformational energy of some arylazo benzothia- zine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and A.	
Jurlewicz	252 (2000) 289
The solvent influence on the electrochemical transfer of divalent ions, O. Pecina and W. Schmickler	252 (2000) 349
The electron localization function description of aromaticity in five-membered rings,	
D.B. Chesnut and L.J. Bartolotti	253 (2000) 1
The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,	
J. Kawai, M. Takahashi, AM. Vlaicu, H. Adachi and T. Mukoyama	253 (2000) 27
Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martín Negri and P.F. Aramendía	253 (2000) 249
Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems:	
ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	253 (2000) 313
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000) 25
E. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	234 (2000) 23

Optical transitions from the chlorine $\theta_u^+(^3P_2)$ ion-pair state, N.K. Bibinov, A.A. Fateev,	
D.B. Kokh, E.V. Lugovoj and A.M. Pravilov Direct correlation method for OH, NH and CH local modes: vibrational overtone	254 (2000) 89
spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenedia-	****
mine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000) 169
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.	254 (2000) 187
Santini and R.S. Cataliotti Kinetic modelling of radiative reacting gas flow under strong nonequilibrium	254 (2000) 337
conditions, E.V. Kustova and A. Chikhaoui Algebraic approach to the potential energy surface for the electronic ground state of	255 (2000) 59
ozone, Y. Zheng and S. Ding Photodissociation spectroscopy of ClCN in the vacuum ultraviolet region, K. Kanda,	255 (2000) 217
M. Kono, T. Nagata, A. Hiraya, K. Tabayashi and K. Shobatake Hartree–Fock crystal orbital calculation on sodium-intercalated fullerites C ₆₀ Na ₁₀ and	255 (2000) 369
C ₆₀ Na ₁₁ , E.B. Starikov Prediction of pure electric-dipole two-photon absorption circular dichroism in	256 (2000) 149
lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman Determination of population, orientation and alignment of symmetric top molecule using laser-induced fluorescence, SL. Cong, KL. Han, GZ. He and	256 (2000) 207
NQ. Lou	256 (2000) 225
Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic \widetilde{B} state, A. Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H.	256 (2000) 220
Baumgärtel Analysis of torsion-rotational transitions in the first three torsional states of CH ₃ OD, I.	256 (2000) 239
Mukhopadhyay and YB. Duan	257 (2000) 91
High resolution near infrared spectrum of solid nitrogen, pure and doped with carbon dioxide, F. Legay and N. Legay-Sommaire	257 (2000) 103
The pair density description of aromaticity in some substituted cyclopentadienyl systems: a comparison of AIM and ELF bonding descriptors, D.B. Chesnut and L.J.	
Bartolotti An experimental and theoretical study of the HNCO ⁺ ion, S. Wilsey, S.E. Thomas and	257 (2000) 175
J.H.D. Eland State selected reactions of krypton ions with methane, A. Kok, P.A.Z. van	258 (2000) 21
Emmichoven and A. Niehaus The structure of water from 25°C to 457°C: comparison between neutron scattering and	258 (2000) 47
molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson	258 (2000) 109
Anomalous X-ray diffraction studies of hydration effects in concentrated aqueous	
electrolyte solutions, S. Ramos, A.C. Barnes, G.W. Neilson and M.J. Capitan Thomas-Reiche-Khun populations in X-CH ₃ and X-C ₂ H ₅ series of molecules, M.E.	258 (2000) 171
Zitto, M.C. Caputo, M.B. Ferraro and P. Lazzeretti Eigenvalue spectrum of the survival probability of excitation in nonradiative energy transport, E.N. Bodunov, M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G.	259 (2000) 1
Martinho Singularities in the Hamiltonian at electronic degeneracies, A.J.C. Varandas and Z.R.	259 (2000) 49
Xu	259 (2000) 173

)3

)9

, , , , , , , , , , , , , , , , , , , ,	
Conical intersections induced by repulsive ${}^1\pi\sigma^*$ states in planar organic molecules: malonaldehyde, pyrrole and chlorobenzene as photochemical model systems, A.L.	
Sobolewski and W. Domcke	259 (2000) 181
Conical intersections and photoreactions of 2H-azirines, C. Bornemann and M.	
Klessinger	259 (2000) 263
On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, O. Plashkevych, T. Privalov,	
H. Ågren, V. Carravetta and K. Ruud	260 (2000) 11
Structure and ground and first electronic excited state vibrational modes of the ethyl-paminobenzoate conformers, A. Longarte, J.A. Fernández, I. Unamuno and F.	
Castaño Semi-empirical study of chain conformation and absorption spectra of polyanilines:	260 (2000) 83
size, solvent and disorder effects, Z.T. de Oliveira and M.C. dos Santos	260 (2000) 95
The photoabsorption and constant ionic state spectroscopy of vinylbromide, A.	200 (2000) 75
Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann, H.W. Jochims and H.	
Baumgrtel	260 (2000) 237
Ab initio calculation for inner reorganization energy of gas-phase electron transfer in	
organic molecule-ion systems, XY. Li, J. Tong and FC. He	260 (2000) 283
Vibronic interactions in {6} and {18}hetero(A,B)annulenes, M. Tachibana and K.	260 (2000) 202
Yoshizawa Hopfield neural network model for calculating the potential energy function from	260 (2000) 303
second virial data, J.P. Braga, M.B. de Almeida, A.P. Braga and J.C. Belchior The effect of carbonyl complexation on highly exothermic vanadium oxidation	260 (2000) 347
reactions, M.J. McQuaid and J.L. Gole	260 (2000) 367
-diatomic	
Photodesorption of NO from a metal surface: quantum dynamical implications of a two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce	251 (2000) 51
The predissociation dynamics of vibrational eigenstates in the $A^2\Sigma^+$ state of HBr ⁺ ions: numerical solution of coupled time-dependent Schrödinger equations, M.V.	
Korolkov and KM. Weitzel	252 (2000) 209
Magnetic fluorescence quenching of the NO β(0-9) transition, V.I. Makarov, I.V.	
Khmelinskii, S.A. Kochubei and V.N. Ishchenko	252 (2000) 379
Nuclear quadrupole coupling constant of ²¹ Ne in the neon dimer and its influence on	
the T_1 NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and M. Jaszuński	253 (2000) 183
Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler, E.E.	255 (2000) 165
Gooch, J.L. Dial and S.K. Knudson	253 (2000) 219
Electronic states of CF ⁺ , I.D. Petsalakis and G. Theodorakopoulos	254 (2000) 181
Broadening and shifting coefficients of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure	
H ₂ : coupled states and semiclassical calculations. Comparison with experiments, X.	
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Laser-induced amplified spontaneous emission from the 3d and nf Rydberg states of	255 (2000) 270
NO, Y. Ogi, M. Takahashi, K. Tsukiyama and R. Bersohn Theoretical study of the electronic structure of the LiRb and NaRb molecules, M.	255 (2000) 379
Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M.	
Aubert-Frécon	256 (2000) 1
	,,

ALLE AND CARLES OF THE CARLES	
Ab initio calculations of the electronic states of KRb, S.J. Park, Y.J. Choi, Y.S. Lee and GH. Jeung	257 (2000) 135
Dispersive photoelectron spectroscopy of the ungerade Rydberg states of Xe ₂ near	237 (2000) 133
Xe*(6p,5d), D.M. Mao, X.K. Hu, Y.J. Shi and R.H. Lipson	257 (2000) 253
The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1	20. (2000) 200
state of Cd-Ar, G.D. Roston and M.S. Helmi	258 (2000) 55
Quasi-classical trajectory simulations of C + NO crossed molecular beam experiments,	
S. Andersson, N. Marković and G. Nyman	259 (2000) 99
The geometric phase effect in chemical reactions, S. Adhikari and G.D. Billing	259 (2000) 149
-small polyatomics	
Electronic and structural properties of CaH ₂ : an ab initio Hartree–Fock study, A. El	
Gridani and M. El Mouhtadi	252 (2000) 1
Theoretical spectroscopic data of the HO ₂ ⁺ ion, J.M. Robbe, M. Monnerville, G. Cham-	
baud, P. Rosmus and P.J. Knowles	252 (2000) 9
Time-dependent quantum dynamics study of reactive scattering of the HD + CN system	
in the potential averaged 5D model, Y. Zhang, Z. Tan, H. Zhang, Q. Zhang and	
J.Z.H. Zhang	252 (2000) 191
An experimental and theoretical study of the valence shell photoelectron spectrum of	
bromobenzene, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K.	
Siegbahn, A.W. Potts and W. von Niessen	252 (2000) 257
Transition intensities in rare gas triatomic ions: DIM versus point-charge approxima-	252 (2000) 201
tion, F.Y. Naumkin	252 (2000) 301
Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and M.F. Gelin	252 (2000) 323
Quantitative studies of the photoabsorption of carbonyl sulphide in the valence-shell, S	232 (2000) 323
2p, 2s and C 1s inner-shell regions (4–360 eV) by dipole electron impact	
spectroscopies, R. Feng, G. Cooper and C.E. Brion	252 (2000) 359
The electron localization function description of aromaticity in five-membered rings,	
D.B. Chesnut and L.J. Bartolotti	253 (2000) 1
Observation of a bottleneck in the vibrational relaxation of liquid bromoform,	
M.A.F.H. van den Broek and H.J. Bakker	253 (2000) 157
Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted	
geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas	253 (2000) 323
Energy dependences of fragment ion yields from acetone photoexcited in the C1s and	
Ols transition regions, I.H. Suzuki and N. Saito	253 (2000) 351
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	
CO ₂ + H ₂ → HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud- Dandine and A. Sevin	254 (2000) 00
Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G.	254 (2000) 99
Baranović	254 (2000) 151
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000) 187
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR	
matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination	, , , , , , , , , , , , , , , , , , , ,
channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	
North	254 (2000) 309

i3

1 9

Study of electron polarization and correlation effects in resonant and back-	
ground electron scattering off CF ₃ Cl, T. Beyer, B.M. Nestmann and S.D.	
Peyerimhoff Ground and excited states of the Ne ₃ ⁺ molecule, J. Urban, P. Mach, J. Mášik, I. Hubač	255 (2000) 1
and V. Staemmler	255 (2000) 15
The nuclear spin-spin coupling constants in methanol and methylamine: geometry and	200 (2000) 10
solvent effects, M. Pecul and J. Sadlej	255 (2000) 137
Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species,	255 (2000) 205
N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews Dipole (e,e+ion) coincidence studies of the ionic photofragmentation and photoioniza-	255 (2000) 205
tion of carbonyl sulfide in the valence shell and S 2p, 2s and C 1s inner shell regions	
(10–300 eV), R. Feng, G. Cooper, Y. Sakai and C.E. Brion	255 (2000) 353
Reactant-product decoupling approach to state-to-state reactive scattering H+DH, S.	
Zhang, Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang	255 (2000) 397
Systematic computational study of the geometrical dependence of deuterium quadru-	
pole interaction parameters in an O ² H···O=C hydrogen bonded system, G.W. Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, DY.	230 (2000) 139
Hwang and A.M. Mebel	256 (2000) 169
A comparison of the oxygen 1s photoabsorption spectra of SO ₂ and NO ₂ , A. Jürgensen	
and R.G. Cavell	257 (2000) 123
A new intermolecular potential energy surface for carbon dioxide from ab initio calculations, S. Bock, E. Bich and E. Vogel	257 (2000) 147
Generalized oscillator strengths for inner-shell excitation of SF ₆ recorded with a high-	257 (2000) 147
performance electron energy loss spectrometer, I.G. Eustatiu, J.T. Francis, T.	
Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P. Hitchcock	257 (2000) 235
About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine	
structure and its vibrational analysis, R. Locht, B. Leyh, A. Hoxha, D. Dehareng,	257 (2000) 202
H.W. Jochims and H. Baumgärtel The radial distribution functions of water and ice from 220 to 673 K and at pressures up	257 (2000) 283
to 400 MPa, A.K. Soper	258 (2000) 121
Production processes of H(D) atoms in the reactions of NO($A^2\Sigma^+$) with C_2H_2 , C_2H_4 ,	
H ₂ O, and their isotopic variants, H. Umemoto, N. Terada, K. Tanaka, T.	
Takayanagi, Y. Kurosaki and K. Yokoyama	259 (2000) 39
Quantum and semiclassical dynamics of the Franck-Condon wave packet on the coupled potential surfaces of the $\widetilde{X}^2A'/\widetilde{A}^2A'$ conical intersection, F. Santoro, C.	
Petrongolo, G. Granucci and M. Persico	259 (2000) 193
Nonadiabatic wave packet dynamics on the coupled $\tilde{X}^2A_1/\tilde{A}^2B_2$ electronic states of	257 (2000) 175
NO ₂ based on new ab initio potential energy surfaces, S. Mahapatra, H. Köppel,	
L.S. Cederbaum, P. Stampfuß and W. Wenzel	259 (2000) 211
Photodynamics of ethylene: ab initio studies of conica! intersections, M. Ben-Nun and	250 (2000) 227
T.J. Martínez Orbital imaging for the valence shell of sulphur dioxide: comparison of EMS	259 (2000) 237
measurements with near Hartree–Fock limit and density functional theory, R. Feng,	
Y. Sakai, Y. Zheng, G. Cooper and C.E. Brion	260 (2000) 29
The equilibrium N-H bond length, J. Demaison, L. Margulès and J.E. Boggs	260 (2000) 65
An extended SU(2) model for coupled Morse oscillators, M. Carvajal, R. Lemus, A.	260 (2000) 105
Frank, C. Jung and E. Ziemniak	260 (2000) 105

Photodissociation dynamics of CH ₂ BrCl at 234 nm, SH. Lee, YJ. Jung and KH.	
Jung	260 (2000) 143
Impulsive IR-multiphoton dissociation of acrolein: observation of non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR fluorescence	
spectroscopy, P.K. Chowdhury Temperature dependent photoabsorption cross sections of allene and methylacetylene	260 (2000) 151
in the VUV-UV region, F.Z. Chen, D.L. Judge and C.Y.R. Wu Vertical triple ionization of ethyne molecules in triple-electron-transfer collisions with	260 (2000) 215
O ²⁺ beam ions, N. Jeffreys, D.E. Parry and F.M. Harris UV, VUV and soft X-ray photoabsorption of dimethyl ether by dipole (e,e)	260 (2000) 295
spectroscopies, R. Feng, G. Cooper and C.E. Brion	260 (2000) 391
-aromatics	
The electron localization function description of aromaticity in five-membered rings,	
D.B. Chesnut and L.J. Bartolotti	253 (2000) 1
Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene	
and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar A systematic investigation of the influence of Cooper minima on the photoionisation	253 (2000) 59
dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson,	
R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen	253 (2000) 133
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular	233 (2000) 133
dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra-	(
phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
A study of the molecular structure and spectroscopic properties of benzo- and pyrido-	(2.2.7)
tetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell	254 (2000) 375
An experimental and theoretical study of the valence shell photoelectron spectrum of the	
chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland,	
M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von Niessen	254 (2000) 385
Methylation effects on the collisional quenching of vibrationally excited benzene	
derivatives by unexcited parent molecules, S.Y. Bae, IJ. Lee and J. Park	255 (2000) 103
Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate	
methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A.	
Costela, I. García-Moreno, R. Sastre and F.J. Duarte	256 (2000) 125
Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin	256 (2000) 127
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach	256 (2000) 137
toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J.	
Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
Electroabsorption spectroscopy of distyrylbenzene derivatives, P.A. Lane, H. Mellor,	230 (2000) 209
S.J. Martin, T.W. Hagler, A. Bleyer and D.D.C. Bradley	257 (2000) 41
The pair density description of aromaticity in some substituted cyclopentadienyl	257 (2000) 41
systems: a comparison of AIM and ELF bonding descriptors, D.B. Chesnut and L.J.	
Bartolotti	257 (2000) 175
Optimization of the molecular hyperpolarizability for second harmonic generation in	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
chiral media, V. Ostroverkhov, O. Ostroverkhova, R.G. Petschek, K.D. Singer, L.	
Sukhomlinova, R.J. Twieg, SX. Wang and L.C. Chien	257 (2000) 263

200	7.5
The lowest energy Frenkel and charge-transfer excitons in quasi-one-dimensional structures: application to MePTCDI and PTCDA crystals, M. Hoffmann, K. Schmidt, T. Fritz, T. Hasche, V.M. Agranovich and K. Leo	258 (2000) 73
Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV photon energy range, M. Schwell, F.v. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H.	260 (2000) 261
Baumgrtel and S. Leach Effect of solvent polarizability on dual fluorescence of <i>EE</i> -1-phenyl,4-(1'-pyrenyl)-1,3-	260 (2000) 261
butadiene, E. Marri, G. Galiazzo, U. Mazzucato and A. Spalletti	260 (2000) 383
-other large	
Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V.	252 (2000) 41
Litvinyuk, Y. Zheng and C.E. Brion Tunneling splittings in vibrational spectra of non-rigid molecules, V.A. Benderskii and	253 (2000) 41
E.V. Vetoshkin	257 (2000) 203
Dihydroazulene/vinylheptafulvene photochromism: dynamics of the photochemical ring-opening reaction, J. Ern, M. Petermann, T. Mrozek, J. Daub, K. Kuldová and	
C. Kryschi	259 (2000) 331
Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV photon energy range, M. Schwell, F.v. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H.	
Baumgrtel and S. Leach	260 (2000) 261
Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonucleosides, O.V. Shishkin, A. Pelmenschikov, D.M. Hovorun and J. Leszczynski	260 (2000) 317
 -polymeric and biological Coupling of diffusion and reaction in the process of capillary formation in alginate gel, H. Treml and HH. Kohler Structure-function self-organization in nonequilibrium macromolecular systems, L.N. 	252 (2000) 199
Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik Density functional theory studies of methylated uracil: geometries and energies, C.F.	256 (2000) 45
Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu Correlated ground-state ab initio calculations of polymethineimine, A. Abdurahman,	256 (2000) 275
A. Shukla and M. Dolg	257 (2000) 301
Hydration structure of the α-chymotrypsin substrate binding pocket: the impact of	250 (2000) 415
constrained geometry, C. Carey, YK. Cheng and P.J. Rossky Femtosecond secondary emission arising from the nonadiabatic photoisomerization in	258 (2000) 415
rhodopsin, S. Hahn and G. Stock	259 (2000) 297
Molecular aggregates	
Determination of protonation sites in bases from topological rules, F. Fuster and B. Silvi	252 (2000) 279
Some regularities of vibrational spectra of a weak hydrogen bond: cooperative and 'anticooperative' effects within the framework of an electrostatic model, N.D.	232 (2000) 279
Sokolov and V.A. Savel'ev	252 (2000) 393
Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M.	
Maggini, M. Prato, I. Lamparth and A. Hirsch	253 (2000) 105

Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of	
the surfactant aerosol-OT, A.K. Mandal and M.K. Pal	253 (2000) 115
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Temperature dependence of fast neutral–neutral reactions: a triatomic model study, A.	254 (2000) 51
Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
The study of A(CH ₃ OH) ₁₋₆ (A = Li ⁺ , Na ⁺) in the gas phase based on ab initio calculations, analysis of the solvation process, A. García-Muruais, E.M. Cabaleiro-Lago, J.M. Hermida-Ramón and M.A. Ríos	254 (2000) 109
Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova	254 (2000) 107
and S. Peyerimhoff	254 (2000) 125
Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	
and B. Brutschy	254 (2000) 407
Infrared spectra of BeNO and MgNO in solid argon, G.P. Kushto, F. Ding, B. Liang, X. Wang, A. Citra and L. Andrews	257 (2000) 223
Structural and dynamical behavior of an azide anion in water from ab initio molecular	237 (2000) 223
dynamics calculations, D.A. Yarne, M.E. Tuckerman and M.L. Klein	258 (2000) 163
Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas	258 (2000) 225
Conical intersections, pseudorotation and coherent oscillations in ultrafast photo- dissociation of group-6 metal hexacarbonyls, S.A. Trushin, W. Fuß and W.E.	
Schmid	259 (2000) 313
Intermolecular potential for benzoic acid-water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik and B.M. Rode	260 (2000) 159
Relaxation of photo-excitations in films of oligo- and poly-(<i>para</i> -phenylene vinylene)	200 (2000) 139
derivatives, S.C.J. Meskers, R.A.J. Janssen, J.E.M. Haverkort and J.H. Wolter	260 (2000) 415
-dimers	
Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras-Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat Vibronic model of hyperfine interaction in dimeric mixed-valence clusters, A.V. Palii,	254 (2000) 275
M.I. Belinsky and B.S. Tsukerblat	255 (2000) 51
Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $O^{-2}H\cdots O=C$ hydrogen bonded system, G.W.	(,
Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard	256 (2000) 105
Dispersive photoelectron spectroscopy of the ungerade Rydberg states of Xe ₂ near	256 (2000) 195
Xe*(6p,5d), D.M. Mao, X.K. Hu, Y.J. Shi and R.H. Lipson	257 (2000) 253
Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H.	207 (2000) 200
Matsui and M. Takeshima	258 (2000) 97
-van der Waals molecules	
Ab initio determination of the $C_6H_6\cdots CS_2$ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto	253 (2000) 165

.5

)7

The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1 state of Cd–Ar, G.D. Roston and M.S. Helmi Photoionization studies of C ₂ H ₃ and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D. Scott, F.H. Watson and G.L. Findley Electronic spectroscopy and structures of the van der Waals complexes of α,00-dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer	Subject maes to courses 251-200	11
Ab initio study of the F ₂ (X ² Sg ⁺)-H(² S) van der Waals complex, V. Lukeš, M. Bittererová, V. Laurine and S. Biskupič The interatomic potentials and dipole moments of the excited 1 _u state of Cd-Cd and ³¹ state of Cd-Ar, G.D. Roston and M.S. Helmi Photoionization studies of C ₂ H ₃ and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D. Scott, F.H. Watson and G.L. Findley Electronic spectroscopy and structures of the van der Waals complexes of α.o-dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer -clusters Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shabbazyan and I.E. Perakis Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ····CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄]* clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical study on the sandwich clusters of Na ₀ (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Theoretical study on the sandwich clusters of Na ₀ (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik		256 (2000) 177
The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1 state of Cd–Ar, G.D. Roston and M.S. Helmi Photoionization studies of C ₂ H ₃ and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D. Scott, F.H. Watson and G.L. Findley Electronic spectroscopy and structures of the van der Waals complexes of α,00-dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer	Ab initio study of the $F_2(X^1\Sigma g^+)$ - $H(^2S)$ van der Waals complex, V. Lukeš, M.	257 (2000) 157
Photoionization studies of C,H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D. Scott, F.H. Watson and G.L. Findley Electronic spectroscopy and structures of the van der Waals complexes of α,ω-dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer 260 (2000) -clusters Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shahbazyan and I.E. Perakis Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ···CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄]* clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ * by H ₂ molecules, S. Roszak, P. Babince and J. Leszczynski Theoretical prediction of a carrier fas offect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ * by H ₂ molecules, S. Roszak, P. Babince and J	The interatomic potentials and dipole moments of the excited 1 _u state of Cd–Cd and ³ 1	
Electronic spectroscopy and structures of the van der Waals complexes of α,ω-dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer 260 (2000) -clusters Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shahbazyan and I.E. Perakis Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ····CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄]* clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ * by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karsaik and C. Flytzanis Structure of NaI on pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Coop	Photoionization studies of C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D.	
-clusters Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shahbazyan and I.E. Perakis Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ····CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe₄S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na ₄ (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _m , Li ⁺ Ar _m and Li ⁺ Kr _m clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of Na1 ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity an	Electronic spectroscopy and structures of the van der Waals complexes of α,ω-	
Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanoparticles, T.V. Shahbazyan and I.E. Perakis Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ···CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol–methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li^Ne _m , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydro		200 (2000) 217
Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the C ₆ H ₆ ····CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄]* clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ * by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li*Ne _m , Li*Ar _n and Li*Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle mode	Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanopar-	251 (2000) 27
The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Ab initio determination of the $C_6H_6\cdots CS_2$ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄]* clusters of ferredoxins with highspin $S = 3/2$ ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ * by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of $Na_n(COT)_m$ by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li*Ne _n , Li*Ar _n and Li*Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Transition intensities in rare gas triatomic ions: DIM versus point-charge approxima-	, , , ,
Ab initio determination of the C ₆ H ₆ ····CS ₂ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of Na1 ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid-water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		252 (2000) 301
A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		252 (2000) 337
Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol–methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid-water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		253 (2000) 165
interaction potential, B. Balta and F.A. Gianturco Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp	253 (2000) 295
Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid-water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	interaction potential, B. Balta and F.A. Gianturco	254 (2000) 203
Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S ₀ and S ₁ states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	
Spangenberg and A. Westphal Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Determination of the structures and barriers to hindered internal rotation of the	254 (2000) 215
spin $S = 3/2$ ground state, M.I. Belinsky Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GH_3^+ by H_2 molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of $Na_n(COT)_m$ by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF_2 crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li^+Ne_n , Li^+Ar_n and Li^+Kr_n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Spangenberg and A. Westphal	254 (2000) 349
chambers, A.L. Itkin New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		255 (2000) 23
New phenomena revealed by quantum chemical studies – the shellvation of GeH ₃ ⁺ by H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Eine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		256 (2000) 61
Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional method, JG. Han, WM. Pang and YY. Shi Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	New phenomena revealed by quantum chemical studies - the shellvation of GeH ₃ ⁺ by	
Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W. Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Theoretical study on the sandwich clusters of Na _n (COT) _m by density functional	
Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E. Froudakis, S.C. Farantos and M. Velegrakis Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Fine level splitting of aggregate neodymium centers in CaF2 crystals, V.V. Fedorov, W.	
Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T. Hynes Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Mass spectra and theoretical modeling of Li ⁺ Ne _n , Li ⁺ Ar _n and Li ⁺ Kr _n clusters, G.E.	
Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas Intermolecular potential for benzoic acid—water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik	Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T.	258 (2000) 13
Intermolecular potential for benzoic acid-water based on the test-particle model and statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik		258 (2000) 201
	Intermolecular potential for benzoic acid-water based on the test-particle model and	258 (2000) 225
		260 (2000) 159

-complexes	
Density functional study of electronic, magnetic and hyperfine properties of $[M(CN)_5NO]^{2-}$ (M = Fe, Ru) and reduction products, J.A. Gómez and D. Guenzburger	253 (2000) 73
Q-Band single-crystal EPR study and molecular orbital calculations of [(C ₆ H ₅) ₄ As] [Re ^{VI} NCl ₄ /Re ^V OCl ₄], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and	233 (2000) 73
R. Kirmse A density functional study of H ₂ O–OClO, (H ₂ O) ₂ –OClO and H ₂ O–ClOO complexes, S.	253 (2000) 171
Aloisio and J.S. Francisco Ab initio study of $M(CH_3CN)_n$ clusters $(M = Li^+, Na^+, Mg^{2+})$ in the gas phase, E.M.	254 (2000) 1
Cabaleiro-Lago and M.A. Ríos Semiempirical modeling free energy surfaces for proton transfer in polar aprotic	254 (2000) 11
solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Density functional calculations on simple carbonyl bases: protonation and hydrogen bond formation with water, A.K. Chandra, M.T. Nguyen and T. Zeegers-	
Huyskens Triplet sublevels of metal organic complexes – temperature dependence of spin–lattice	255 (2000) 149
relaxation, J. Strasser, H.H.H. Homeier and H. Yersin Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclote-	255 (2000) 301
tradecane)chromium(III) nitrate, JH. Choi Theoretical study of cation– π interactions of the metal complex cation, $[Co(NH_3)_6]^{3+}$,	256 (2000) 29
with ethylene and acetylene, S.D. Zarić Laser flash photolysis of $IrCl_6^2$ in aqueous solutions, E.M. Glebov, V.F. Plyusnin, N.V.	256 (2000) 213
Tkachenko and H. Lemmetyinen	257 (2000) 79
Free radicals (incl. hydronium and muonium)	
Calculation of CIDNP field dependences in biradicals in the photolysis of large-ring cycloalkanones, A.V. Popov, P.A. Purtov and A.V. Yurkovskaya	252 (2000) 83
Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission	252 (2000) 05
spectroscopy T Kimura M Sumimoto S Sakaki H Fujimoto V Hashimoto and	
spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki Kingtics of the reactions of ECOOD, radicals with F atoms and F. M.P. Radenes, F.	253 (2000) 125
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri	253 (2000) 125 253 (2000) 205
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N.	253 (2000) 205
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (A B	
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (A B ₁ (0,7,0)) by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño	253 (2000) 205
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (A	253 (2000) 205 253 (2000) 231 254 (2000) 77
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (A B ₁ (0,7,0)) by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W. North Quantum beats in recombination of spin-correlated radical ion pairs with equivalent	253 (2000) 205 253 (2000) 231
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (¹B ₁ (0,7,0)) by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W. North Quantum beats in recombination of spin-correlated radical ion pairs with equivalent protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N. Molin	253 (2000) 205 253 (2000) 231 254 (2000) 77
S. Matsuzaki Kinetics of the reactions of FC(O)O ₂ radicals with F atoms and F ₂ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin The collisional removal of the carbene CCl ₂ (X(0,0,0)) and CCl ₂ (¹B ₁ (0,7,0)) by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W. North Quantum beats in recombination of spin-correlated radical ion pairs with equivalent protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N.	253 (2000) 205 253 (2000) 231 254 (2000) 77 254 (2000) 309

Li cation–aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W.	
Dwyer	256 (2000) 37
Primary steps of an electron–proton reaction in aqueous electrolyte solutions, Y.	250 (2000) 57
Gauduel and H. Gelabert	256 (2000) 333
Quasi-classical trajectory simulations of C + NO crossed molecular beam experiments,	250 (2000) 555
S. Andersson, N. Marković and G. Nyman	259 (2000) 99
Nonadiabatic wave packet dynamics on the coupled $\tilde{X}^2A_1/\tilde{A}^2B_2$ electronic states of	239 (2000) 99
NO ₂ based on new ab initio potential energy surfaces, S. Mahapatra, H. Köppel,	
L.S. Cederbaum, P. Stampfuß and W. Wenzel	259 (2000) 211
Recombination yield of geminate radical pairs in high magnetic fields: general	239 (2000) 211
results and application to free diffusion, M.J. Hansen, A.A. Neufeld and	
J.B. Pedersen	260 (2000) 125
J.B. Tedelsen	200 (2000) 123
Quasiparticles (incl. excitons)	
Photoemission linewidths narrower than the quasiparticle inverse lifetime, TC. Chiang	251 (2000) 133
q-maps and a second method at the contract of	(2000) 200
Ions and charge carriers	
A universal Gaussian basis set for positive and negative ions from H through Xe, F.E.	
Jorge and M.L. Franco	253 (2000) 21
Influence of geminate recombination kinetics on the shape of low field MARY line,	
Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin	253 (2000) 231
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	
CO ₂ + H ₂ → HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud-	
Dandine and A. Sevin	254 (2000) 99
Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo	
envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W.	
Dwyer	256 (2000) 37
A proper mobility formula for large, heavy particles in gases in any regime, L. Ferrari	257 (2000) 63
Solvent effect on Sr ²⁺ to Ca ²⁺ ion mutation: Monte Carlo simulation study, HS. Kim	257 (2000) 183
Quantum dynamics of model proton-coupled electron transfer reactions, S. Shin and	
SI. Cho	259 (2000) 27
Suppose decides accomplise (in all many positions and a many transpose	
Supramolecular assemblies (incl. nanoparticles and nanostructures) Electron dynamics and surface plasmon resonance nonlinearities in metal nanoparti-	
cles, N. Del Fatti, F. Valleé, C. Flytzanis, Y. Hamanaka and A. Nakamura	251 (2000) 215
cies, N. Dei Fatti, F. Vaniee, C. Flytzanis, T. Hamanaka and A. Nakamura	251 (2000) 215
Liquid-liquid and liquid-solid interfaces	
Relaxational dynamics of water molecules at protein surface, S. Dellerue and MC.	
Bellissent-Funel	258 (2000) 315
Hydration structure of the α-chymotrypsin substrate binding pocket: the impact of	, , , , , , , ,
constrained geometry, C. Carey, YK. Cheng and P.J. Rossky	258 (2000) 415
Nature of collagen-water hydration forces: a problem in water structure, G.E.	
Walrafen and YC. Chu	258 (2000) 427
Biological assemblies, cells and organelles	
Nature of collagen-water hydration forces: a problem in water structure, G.E.	250 (2000) 425
Walrafen and YC. Chu	258 (2000) 427

Proteins

Some remarks on the application of relaxation techniques to chemical equilibria, M. Galán and G. Angulo

254 (2000) 329

Exchange variation of zero-field splittings in $[Fe_4S_4]^+$ clusters of ferredoxins with highspin S = 3/2 ground state, M.I. Belinsky Dielectric relaxations of collagen and elastin in the dehydrated state, V. Samouillan, A.

255 (2000) 23

Lamure and C. Lacabanne DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-N'-methylamide for n = 1-20,

255 (2000) 259

M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai Relaxational dynamics of water molecules at protein surface, S. Dellerue and M.-C.

256 (2000) 15 258 (2000) 315

New perspectives on hydrophobic effects, G. Hummer, S. Garde, A.E. García and L.R. Pratt

258 (2000) 349

Nucleic acids

Bellissent-Funel

The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán

253 (2000) 13

The role of water in B-DNAs B_I to B_{II} conformer substates interconversion: a combined study by calorimetry, FT-IR spectroscopy and computer simulation, A. Pichler, S. Rüdisser, R.H. Winger, K.R. Liedl, A. Hallbrucker and E. Mayer

258 (2000) 391

Phenomena

Molecular structure

A theoretical study of plutonium diketone complexes for solvent extraction, L. Gagliardi, N.C. Handy, C.-K. Skylaris and A. Willetts

252 (2000) 47

The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán

253 (2000) 13

A theoretical exploratory study of low-energy (1–2 eV) electron catalysis in the $CO_2 + H_2 \rightarrow HCOOH$ gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud-Dandine and A. Sevin

254 (2000) 99

Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova and S. Peyerimhoff

254 (2000) 125

Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini

254 (2000) 187

Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani

254 (2000) 215

Activation of CO₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and Q.-Z. Qin

254 (2000) 231

Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron

254 (2000) 267

Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal

254 (2000) 349

A study of the molecular structure and spectroscopic properties of benzo- and pyridotetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell

254 (2000) 375

Subject index to volumes 251–260	8	81
Ground and excited states of the Ne ₃ ⁺ molecule, J. Urban, P. Mach, J. Mášik, I. Hubač and V. Staemmler	255 (2000) 1	15
Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-dichloropropane in carbon tetrachloride, S. Madurga, J.C. Paniagua and E.		
Vilaseca The nuclear spin-spin coupling constants in methanol and methylamine: geometry and	255 (2000) 12	23
solvent effects, M. Pecul and J. Sadlej	255 (2000) 13	37
Density functional calculations on simple carbonyl bases: protonation and hydrogen bond formation with water, A.K. Chandra, M.T. Nguyen and T. Zeegers-	255 (2000) 1	40
Huyskens Infrared spectra of monomeric L-alanine and L-alanine-N-d ₃ zwitterions isolated in a	255 (2000) 14	19
KBr matrix, X. Cao and G. Fischer	255 (2000) 19	95
Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species,	200 (2000) 1.	
N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews	255 (2000) 20	05
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M.		
Aubert-Frécon	256 (2000)	1
Theoretical study of the infrared and ultraviolet spectrum of the radical F ₂ CN, H. Dupin, I. Baraille, C. Larrieu and A. Dargelos	256 (2000)	7
DFT studies on helix formation in N-acetyl-(L -alanyl) _n -N'-methylamide for $n = 1-20$,	256 (2000)	7
M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and		
S. Suhai	256 (2000)	15
New phenomena revealed by quantum chemical studies - the shellvation of GeH ₃ ⁺ by		
H ₂ molecules, S. Roszak, P. Babinec and J. Leszczynski	256 (2000) 1	77
Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou	256 (2000) 1	85
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E.		
Alikhani and J.P. Perchard	256 (2000) 1	95
Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer	256 (2000) 2	051
Density functional theory studies of methylated uracil: geometries and energies, C.F.	256 (2000) 2	.51
Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu	256 (2000) 2	275
Isomerism of the covalent anion of the dimer of uracil and 1-methyl-cytosine: ab initio	(
study, I. Al-Jihad, J. Smets and L. Adamowicz	257 (2000) 1	67
Correlated ground-state ab initio calculations of polymethineimine, A. Abdurahman,		
A. Shukla and M. Dolg	257 (2000) 3	
Cooperativity and hydrogen bonding network in water clusters, S.S. Xantheas	258 (2000) 2	225
Ab initio study of the reaction mechanism of singlet and triplet N ₂ O and their	250 (2000)	00
intersystem crossing, DY. Hwang and A.M. Mebel Cytosine anions: abinitio study, D.M.A. Smith, A.F. Jalbout, J. Smets and L.	259 (2000)	89
Adamowicz	260 (2000)	45
Substituent effects on the intramolecular proton transfer in the ground and	200 (2000)	45
lowest-lying singlet excited states of salicylaldimine, M. Forés, M. Duran and		
M. Solà	260 (2000)	53
The equilibrium N-H bond length, J. Demaison, L. Margulès and J.E. Boggs	260 (2000)	65
An extended SU(2) model for coupled Morse oscillators, M. Carvajal, R. Lemus, A.		
Frank, C. Jung and E. Ziemniak	260 (2000) 1	105

Vibrations and rotations of molecules	
Reassignment of ground and first excited state vibrations in phenol, W. Roth, P. Imhof,	
M. Gerhards, S. Schumm and K. Kleinermanns	252 (2000) 247
A classical algebraic approach to the bend motion of acetylene: the formalism by two	
coupled cosets, G. Wu	252 (2000) 315
Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave	
number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa,	
C. Abematsu, S. Yajima and K. Ishii	253 (2000) 331
A density functional study of H ₂ O-OClO, (H ₂ O) ₂ -OClO and H ₂ O-ClOO complexes, S.	
Aloisio and J.S. Francisco	254 (2000) 1
Direct correlation method for OH, NH and CH local modes: vibrational overtone	
spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenedia-	
mine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000) 169
Activation of CO2 by Zr atom. Matrix-isolation FTIR spectroscopy and density	
functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin	254 (2000) 231
Broadening and shifting coefficients of Raman isotropic $Q(j)(j = 0, 1, 2)$ lines for pure	
H ₂ : coupled states and semiclassical calculations. Comparison with experiments,	
X. Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes	
in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.	
Santini and R.S. Cataliotti	254 (2000) 337
Semiclassical description of purely rotational recurrences for collisionless asymmetric	
top molecules: new results, M.F. Gelin, V.A. Tolkachev and A.P. Blokhin	255 (2000) 111
Infrared spectra of monomeric L-alanine and L-alanine-N-d3 zwitterions isolated in a	
KBr matrix, X. Cao and G. Fischer	255 (2000) 195
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M.	
Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M.	
Aubert-Frécon	256 (2000) 1
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P.	
Postorino	256 (2000) 117
Theoretical investigation on the potential energy surface for the reactions of B, Al and	
Ga with NO, L. Zhang and M. Zhou	256 (2000) 185
Analysis of torsion-rotational transitions in the first three torsional states of CH3OD, I.	
Mukhopadhyay and YB. Duan	257 (2000) 91
Quasi-classical dynamics and vibrational kinetics of $N + N_2(v)$ system, F. Esposito, M.	
Capitelli and C. Gorse	257 (2000) 193
Structural and dynamical behavior of an azide anion in water from ab initio molecular	
dynamics calculations, D.A. Yarne, M.E. Tuckerman and M.L. Klein	258 (2000) 163
Reorientational motion and hydrogen-bond stretching dynamics in liquid water, H.J.	
Bakker, S. Woutersen and HK. Nienhuys	258 (2000) 233
Generalized frequency spectra of water at both sides of the freezing transition, J.	
Dawidowski, F.J. Bermejo, C. Cabrillo and S.M. Bennington	258 (2000) 247
Vibrational corrections to linear and nonlinear static electric properties of polyatomic	
molecules at non-optimum reference geometry, V.E. Ingamells, M.G. Papadopoulos	
and A.J. Sadlej	260 (2000) 1
Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the	
ground state and vibrational analysis, H. Okamoto, H. Inishi, Y. Nakamura, S.	
Kohtani and R. Nakagaki	260 (2000) 193

Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonu-	
cleosides, O.V. Shishkin, A. Pelmenschikov, D.M. Hovorun and J. Leszczynski	260 (2000) 317
Electronic structure and states	
Theory of inelastic lifetimes of low-energy electrons in metals, P.M. Echenique, J.M.	
Pitarke, E.V. Chulkov and A. Rubio	251 (2000) 1
Femtosecond two-photon photoemission studies of image-potential states, T. Fauster,	
C. Reuß, I.L. Shumay and M. Weinelt	251 (2000) 111
Influence of Xe adlayer morphology and electronic structure on image-potential state	
lifetimes of Ru(0001), W. Berthold, U. Höfer, P. Feulner and D. Menzel	251 (2000) 123
Photoemission linewidths narrower than the quasiparticle inverse lifetime, TC. Chiang	251 (2000) 133
Ultrafast electron and lattice dynamics in semiconductors at high excited carrier	
densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur	251 (2000) 167
Theoretical spectroscopic data of the HO ₂ ⁺ ion, J.M. Robbe, M. Monnerville, G. Cham-	
baud, P. Rosmus and PJ. Knowles	252 (2000) 9
The attractive quartet potential energy surface for the $CH_3C(a^4A_2)$ + CO reaction, H.	
Hou, B. Wang and Y. Gu	252 (2000) 17
A theoretical study of plutonium diketone complexes for solvent extraction, L.	
Gagliardi, N.C. Handy, CK. Skylaris and A. Willetts	252 (2000) 47
An experimental and theoretical study of the valence shell photoelectron spectrum of	
bromobenzene, D.M.P. Holland, D. Edvardsson, L. Karlson, R. Maripuu, K.	0.50 (0.000) 0.55
Siegbahn, A.W. Potts and W. von Niessen	252 (2000) 257
A universal Gaussian basis set for positive and negative ions from H through Xe, F.E.	0.50 (0.000) 0.4
Jorge and M.L. Franco	253 (2000) 21
The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,	
J. Kawai, M. Takahashi, AM. Vlaicu, H. Adachi and T. Mukoyama	253 (2000) 27
Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V.	252 (2000) 44
Litvinyuk, Y. Zheng and C.E. Brion	253 (2000) 41
Vibronic coupling for H ₂ CO and CO ₂ , A.B. Rocha and C.E. Bielschowsky	253 (2000) 51
Density functional study of electronic, magnetic and hyperfine properties of	
$[M(CN)_5NO]^{2-}$ (M = Fe, Ru) and reduction products, J.A. Gómez and D.	252 (2000) 72
Guenzburger	253 (2000) 73
Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission	
spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and	252 (2000) 125
S. Matsuzaki	253 (2000) 125
A systematic investigation of the influence of Cooper minima on the photoionisation	
dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson,	252 (2000) 122
R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen	253 (2000) 133
Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler, E.E.	252 (2000) 210
Gooch, J.L. Dial and S.K. Knudson	253 (2000) 219
Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-	
nitro)- and 1-(3-aminophenyl)-1 <i>H</i> -methanofullerene doped with cobaltocene, P.	252 (2000) 261
Umek, A. Omerzu, D. Mihailović and M. Tokumoto	253 (2000) 361
The collisional removal of the carbone $CCl_2(\widetilde{X}(0,0,0))$ and $CCl_2(\widetilde{A}^1B_1(0,7,0))$ by rare	
gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	254 (2000) 77
Rayo, D. Husain and F. Castaño	254 (2000) 77
Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G. Baranović	254 (2000) 151
Baranovic	254 (2000) 151

04		Subject maex to totalnes 251-200		
	ronic states of CF ⁺ , I.D. Petsalaki	s and G. Theodorakopoulos ts in protonated helium clusters. I. The ab in	254 (2000) 181	
int	eraction potential, B. Balta and F		254 (2000) 203	
fu	nctional studies, L. Zhang, X. Wa	ng, M. Chen and QZ. Qin	254 (2000) 231	
K	arabunarliev and M. Baumgarten	high-spin ground states in ion radicals	254 (2000) 239	
Al	menar, J.M. Clemente-Juan, E. C.	y degenerate mixed valence systems, J.J. Bor oronado, A.V. Palii and B.S. Tsukerblat	254 (2000) 275	
te	raazapentalenes, V. Galasso, D. J	spectroscopic properties of benzo- and pyrones, A. Modelli and M.L. Trudell	254 (2000) 375	
th	e chlorobenzene molecule, A.W.	of the valence shell photoelectron spectrum Potts, D. Edvardsson, L. Karlsson, D.M. Hayes, R. Maripuu, K. Siegbahn and W.	1.P.	
	lessen and excited states of the Ne ₃ ⁺ n	nolecule, J. Urban, P. Mach, J. Mášik, I. Hu	254 (2000) 385 ibač	
an	d V. Staemmler	igs in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with h	255 (2000) 15	
sp	in $S = 3/2$ ground state, M.I. Beli		255 (2000) 23	
M	.I. Belinsky and B.S. Tsukerblat	l vibrational circular dichroism spectra o	255 (2000) 51	
al F	anine in aqueous solution: a de rimand, H. Bohr, K.J. Jalkanen ar	nsity functional theory and RHF study, and S. Suhai	K. 255 (2000) 165	
	odissociation spectroscopy of ClC Kono, T. Nagata, A. Hiraya, K.	N in the vacuum ultraviolet region, K. Ka . Tabayashi and K. Shobatake	nda, 255 (2000) 369	
	r-induced amplified spontaneous e O, Y. Ogi, M. Takahashi, K. Tsul	emission from the 3d and nf Rydberg state kiyama and R. Bersohn	s of 255 (2000) 379	,
K	orek, A.R. Allouche, M. Kobeissi,	ructure of the LiRb and NaRb molecules. A. Chaalan, M. Dagher, K. Fakherddin and	1 M.	
The		ultraviolet spectrum of the radical F ₂ CN	256 (2000) 1 , H.	
	upin, I. Baraille, C. Larrieu and A ree-Fock crystal orbital calculatio	 Dargelos n on sodium-intercalated fullerites C₆₀Na₁₀ 	256 (2000) 7 and	
	₆₀ Na ₁₁ , E.B. Starikov pretical investigation on the potent	ial energy surface for the reactions of B, Al	256 (2000) 149 and	1
	a with NO, L. Zhang and M. Zho tronic energy dynamics of photo	ou excited ternary Zintl phase LiSbTe ₂ and	256 (2000) 185 the	
	stance estimation between trap si ing and SH. Lee	tes, SG. Kang, WS. Chae, YR. Kim,	JS. 256 (2000) 295	;
p	yridazine, G. Fischer and P. Worn		257 (2000) 1	
	pretical study on the sandwich aethod, JG. Han, WM. Pang an	clusters of $Na_n(COT)_m$ by density function of YY. Shi	onal 257 (2000) 21	
	troabsorption spectroscopy of dis J. Martin, T.W. Hagler, A. Bleyer	tyrylbenzene derivatives, P.A. Lane, H. Mer and D.D.C. Bradley	ellor, 257 (2000) 41	1
	omparison of the oxygen 1s photoa nd R.G. Cavell	bsorption spectra of SO ₂ and NO ₂ , A. Jürge	nsen 257 (2000) 123	3

Subject times to commes 251-200	83
Ab initio calculations of the electronic states of KRb, S.J. Park, Y.J. Choi, Y.S. Lee and	257 (2000) 125
GH. Jeung Generalized oscillator strengths for inner-shell excitation of SF ₆ recorded with a high- performance electron energy loss spectrometer, I.G. Eustatiu, J.T. Francis, T.	257 (2000) 135
Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P. Hitchcock	257 (2000) 235
Dispersive photoelectron spectroscopy of the ungerade Rydberg states of Xe ₂ near Xe [*] (6p,5d), D.M. Mao, X.K. Hu, Y.J. Shi and R.H. Lipson	257 (2000) 253
Optimization of the molecular hyperpolarizability for second harmonic generation in chiral media, V. Ostroverkhov, O. Ostroverkhova, R.G. Petschek, K.D. Singer, L. Sukhomlinova, R.J. Twieg, SX. Wang and L.C. Chien	257 (2000) 263
An experimental and theoretical study of the HNCO+ ion, S. Wilsey, S.E. Thomas and	
J.H.D. Eland Effect of a dissipative environment on the dynamics at a conical intersection, A. Kühl	258 (2000) 21
and W. Domcke	259 (2000) 227
Photodynamics of ethylene: ab initio studies of conical intersections, M. Ben-Nun and T.J. Martínez	250 (2000) 227
Orbital imaging for the valence shell of sulphur dioxide: comparison of EMS measurements with near Hartree-Fock limit and density functional theory, R. Feng,	259 (2000) 237
Y. Sakai, Y. Zheng, G. Cooper and C.E. Brion	260 (2000) 29
Cytosine anions: abinitio study, D.M.A. Smith, A.F. Jalbout, J. Smets and L. Adamowicz Substituent effects on the intramolecular proton transfer in the ground and lowest-lying	260 (2000) 45
singlet excited states of salicylaldimine, M. Forés, M. Duran and M. Solà Semi-empirical study of chain conformation and absorption spectra of polyanilines:	260 (2000) 53
size, solvent and disorder effects, Z.T. de Oliveira and M.C. dos Santos	260 (2000) 95
Temperature dependent photoabsorption cross sections of allene and methylacetylene in the VUV–UV region, F.Z. Chen, D.L. Judge and C.Y.R. Wu	260 (2000) 215
Vertical triple ionization of ethyne molecules in triple-electron-transfer collisions with	200 (2000) 213
O ²⁺ beam ions, N. Jeffreys, D.E. Parry and F.M. Harris	260 (2000) 295
Electric and magnetic properties	
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell	251 (2000) 227
DFT and HF-DFT calculations of ¹⁴ N quadrupole coupling constants in molecules,	, , , , ,
W.C. Bailey Transition intensities in rare gas triatomic ions: DIM versus point-charge approxima-	252 (2000) 57
tion, F.Y. Naumkin	252 (2000) 301
Density functional study of electronic, magnetic and hyperfine properties of $[M(CN)_5NO]^{2-}$ (M = Fe, Ru) and reduction products, J.A. Gómez and D. Guenzburger	253 (2000) 73
Q-Band single-crystal EPR study and molecular orbital calculations of [(C ₆ H ₅) ₄ As]-[Re ^{VI} NCl ₄ /Re ^V OCl ₄], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and	200 (2000) 13
R. Kirmse Nuclear quadrupole coupling constant of ²¹ Ne in the neon dimer and its influence on	253 (2000) 171
the T_1 NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and	
M. Jaszuński The nuclear spin-spin coupling constants in methanol and methylamine: geometry and	253 (2000) 183
solvent effects, M. Pecul and J. Sadlej	255 (2000) 137

Magnetic exchange interaction between π -electron radicals adsorbed on graphites, N.	
Tyutyulkov, F. Dietz and K. Müllen	255 (2000) 223
Optical spectroscopy and crystal-field effects on the paramagnetic susceptibility of rare-earth germanates $GaRGe_2O_7$, $R=Pr$, Nd, C. Cascales, G. Lozano, C. Zaldo and P.	
Porcher	257 (2000) 29
Recombination yield of geminate radical pairs in high magnetic fields: general results and application to free diffusion, M.J. Hansen, A.A. Neufeld and J.B. Pedersen Density functional theory and Hartree–Fock-density functional theory calculations of	260 (2000) 125
¹⁷ O, ³³ S, and ⁷³ Ge quadrupole coupling constants, W.C. Bailey, F.M. Gonzalez and J. Castiglione	260 (2000) 327
Spin splittings	
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S.	
Karabunarliev and M. Baumgarten	254 (2000) 239
Exchange variation of zero-field splittings in [Fe ₄ S ₄] ⁺ clusters of ferredoxins with high-	
spin $S = 3/2$ ground state, M.I. Belinsky	255 (2000) 23
Triplet sublevels of metal organic complexes – temperature dependence of spin–lattice	
relaxation, J. Strasser, H.H.H. Homeier and H. Yersin	255 (2000) 301
Molecular interactions	
Time-dependent quantum dynamics study of reactive scattering of the HD + CN system in the potential averaged 5D model, Y. Zhang, Z. Tan, H. Zhang, Q. Zhang and	
J.Z.H. Zhang	252 (2000) 191
Determination of protonation sites in bases from topological rules, F. Fuster and B. Silvi	252 (2000) 279
Ab initio determination of the $C_6H_6\cdots CS_2$ cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto	253 (2000) 165
Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-	
free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg	253 (2000) 283
Monte Carlo simulation study of solvent effect on Na^+ to Li^+ ion mutation, HS. Kim Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D.	253 (2000) 305
Spangenberg and A. Westphal Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond	254 (2000) 349
association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón	255 (2000) 73
Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-dichloropropane in carbon tetrachloride, S. Madurga, J.C. Paniagua and E. Vilaseca	255 (2000) 123
Algebraic approach to the potential energy surface for the electronic ground state of ozone, Y. Zheng and S. Ding	255 (2000) 217
Reactant-product decoupling approach to state-to-state reactive scattering H+DH, S.	
Zhang, Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang	255 (2000) 397
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino	256 (2000) 115
Systematic computational study of the geometrical dependence of deuterium quadru-	256 (2000) 117
pole interaction parameters in an $O^{-2}H \cdots O=C$ hydrogen bonded system, G.W.	
Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
	(2000) 10)

	01
High resolution study of 1388 cm ⁻¹ CO ₂ vibration by time-domain CARS: spectral exchange and Dicke effect, D.S. Kuznetsov, V.B. Morozov, A.N. Olenin and V.G.	
Tunkin	257 (2000) 117
A new intermolecular potential energy surface for carbon dioxide from ab initio calculations, S. Bock, E. Bich and E. Vogel Ab initio study of the $F_2(X^1\Sigma_{\sigma}^+)$ - $H(^2S)$ van der Waals complex, V. Lukeš, M.	257 (2000) 147
Bittererová, V. Laurinc and S. Biskupič The interatomic potentials and dipole moments of the excited 1_u state of Cd–Cd and 31	257 (2000) 157
state of Cd–Ar, G.D. Roston and M.S. Helmi The radial distribution functions of water and ice from 220 to 673 K and at pressures up	258 (2000) 55
to 400 MPa, A.K. Soper Structure of NaI ion pairs in water clusters, G.H. Peslherbe, B.M. Ladanyi and J.T.	258 (2000) 121
Hynes On the origin of the heat capacity feature of annealed ices and ice clathrates, and	258 (2000) 201
interpreting water's diffusivity in terms of the entropy, G.P. Johari New perspectives on hydrophobic effects, G. Hummer, S. Garde, A.E. García and L.R.	258 (2000) 277
Pratt A recursive Kohn variational algorithm for the Green's operator: application to the T-	258 (2000) 349
matrix, D. Brown Intermolecular potential for benzoic acid-water based on the test-particle model and	259 (2000) 11
statistical mechanical simulations of benzoic acid in aqueous solutions, K. Sagarik and B.M. Rode	260 (2000) 159
Spectral bandshapes and intensities	
Motional effects on optimum coherence transfer in ² H MAS NMR spectroscopy, J.H. Kristensen, G.L. Hoatson and R.L. Vold	252 (2000) 97
Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation, F.Y. Naumkin	252 (2000) 301
Quantitative studies of the photoabsorption of carbonyl sulphide in the valence-shell, S 2p, 2s and C 1s inner-shell regions (4–360 eV) by dipole electron impact	
spectroscopies, R. Feng, G. Cooper and C.E. Brion	252 (2000) 359
Vibronic coupling for H ₂ CO and CO ₂ , A.B. Rocha and C.E. Bielschowsky Dipole (e,e+ion) coincidence studies of the ionic photofragmentation and photoioniza- tion of carbonyl sulfide in the valence shell and S 2p, 2s and C 1s inner shell regions	253 (2000) 51
(10–300 eV), R. Feng, G. Cooper, Y. Sakai and C.E. Brion Spectral density of medium strength H-bonds. Direct damping and intrinsic	255 (2000) 353
anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau	256 (2000) 85
Determination of single-site absorption spectrum in dye-doped disordered materials by double site-selective spectroscopy, Y. Ichino, Y. Kanematsu, A. Kurita and T.	200 (2000)
Kushida Nonadiabatic wave packet dynamics on the coupled $\widetilde{X}^2A_1/\widetilde{A}^2B_2$ electronic states of	259 (2000) 63
NO ₂ based on new ab initio potential energy surfaces, S. Mahapatra, H. Köppel, L.S. Cederbaum, P. Stampfuß and W. Wenzel	259 (2000) 211
Electronic spectroscopy and structures of the van der Waals complexes of α,ω -dihaloalkanes with anthracene, J.C. Hlady and R.P. Steer	260 (2000) 249
UV, VUV and soft X-ray photoabsorption of dimethyl ether by dipole (e,e) spectroscopies, R. Feng, G. Cooper and C.E. Brion	260 (2000) 391

Coupling of electronic and nuclear motion	
Quasi-particle lifetimes on noble metal surfaces studied by ARPES and STM, R.	
Matzdorf	251 (2000) 151
Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y.	253 (2000) 231
Gauduel and H. Gelabert	256 (2000) 333
Vibronic analyses of the lowest singlet-singlet and singlet-triplet band systems of pyridazine, G. Fischer and P. Wormell	257 (2000) 1
About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine structure and its vibrational analysis, R. Locht, B. Leyh, A. Hoxha, D. Dehareng,	
H.W. Jochims and H. Baumgärtel	257 (2000) 283
Quantum dynamics of model proton-coupled electron transfer reactions, S. Shin and SI. Cho	259 (2000) 27
Determination of single-site absorption spectrum in dye-doped disordered materials by double site-selective spectroscopy, Y. Ichino, Y. Kanematsu, A. Kurita and T.	
Kushida	259 (2000) 63
Singularities in the Hamiltonian at electronic degeneracies, A.J.C. Varandas and Z.R. Xu Quantum and semiclassical dynamics of the Franck-Condon wave packet on the coupled potential surfaces of the $\widetilde{X}^2A'/\widetilde{A}^2A'$ conical intersection, F. Santoro, C.	259 (2000) 173
Petrongolo, G. Granucci and M. Persico	259 (2000) 193
A model study of the wavepacket dynamics around a Jahn-Teller conical intersection in	
a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani Nonadiabatic wave packet dynamics on the coupled $\widetilde{X}^2A_1/\widetilde{A}^2B_2$ electronic states of NO ₂ based on new ab initio potential energy surfaces, S. Mahapatra, H. Köppel,	259 (2000) 201
L.S. Cederbaum, P. Stampfuß and W. Wenzel	259 (2000) 211
Photodynamics of ethylene: ab initio studies of conical intersections, M. Ben-Nun and	
T.J. Martínez Femtosecond secondary emission arising from the nonadiabatic photoisomerization in	259 (2000) 237
rhodopsin, S. Hahn and G. Stock	259 (2000) 297
Vibronic interactions in {6} and {18}hetero(A,B)annulenes, M. Tachibana and K.	237 (2000) 277
Yoshizawa	260 (2000) 303
Relaxation of photo-excitations in films of oligo- and poly-(para-phenylene vinylene) derivatives, S.C.J. Meskers, R.A.J. Janssen, J.E.M. Haverkort and J.H. Wolter	260 (2000) 415
Energy transfer processes	
Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in desorption, J.W. Gadzuk	251 (2000) 87
Ultrafast electron and lattice dynamics in semiconductors at high excited carrier densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur	251 (2000) 167
Electron dynamics in metallic nanoparticles, JY. Bigot, V. Halté, JC. Merle and A. Daunois	251 (2000) 181
A classical algebraic approach to the bend motion of acetylene: the formalism by two coupled cosets, G. Wu	252 (2000) 315
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	202 (2000) 515
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek Methylation effects on the collisional quenching of vibrationally excited benzene	254 (2000) 319
derivatives by unexcited parent molecules, S.Y. Bae, IJ. Lee and J. Park	255 (2000) 103

Statistical dynamics in rotationally inelastic gas-surface scattering: dynamical Lie	255 (2000) 252
algebraic method, Y. Zheng, X. Yi, D. Guan and Q. Meng Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon	255 (2000) 273
monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J.W. Rich Quasi-classical dynamics and vibrational kinetics of $N + N_2(v)$ system, F. Esposito, M.	256 (2000) 315
Capitelli and C. Gorse	257 (2000) 193
Eigenvalue spectrum of the survival probability of excitation in nonradiative energy transport, E.N. Bodunov, M.N. Berberan-Santos, E.J. Nunes Pereira and J.M.G. Martinho	259 (2000) 49
Energy dissipation and relaxation processes in deoxy myoglobin after photoexcitation	239 (2000) 49
in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochstrasser Relaxation processes in singlet O ₂ analyzed by laser-induced gratings, W. Hubschmid	259 (2000) 71
and B. Hemmerling	259 (2000) 109
Relaxation of photo-excitations in films of oligo- and poly-(para-phenylene vinylene)	
derivatives, S.C.J. Meskers, R.A.J. Janssen, J.E.M. Haverkort and J.H. Wolter	260 (2000) 415
Molecular photophysical processes	
An experimental and theoretical study of the valence shell photoelectron spectrum of	
bromobenzene, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K.	
Siegbahn, A.W. Potts and W. von Niessen	252 (2000) 257
Quantitative studies of the photoabsorption of carbonyl sulphide in the valence-shell, S 2p, 2s and C 1s inner-shell regions (4–360 eV) by dipole electron impact	
spectroscopies, R. Feng, G. Cooper and C.E. Brion	252 (2000) 359
Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis	252 (2000) 557
and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M.	
Maggini, M. Prato, I. Lamparth and A. Hirsch	253 (2000) 105
Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of	252 (2000) 115
the surfactant aerosol-OT, A.K. Mandal and M.K. Pal A systematic investigation of the influence of Cooper minima on the photoionisation	253 (2000) 115
dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson,	
R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen	253 (2000) 133
Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps	
transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W.	
Rettig	253 (2000) 339
Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions, I.H. Suzuki and N. Saito	252 (2000) 251
Singlet–singlet excited-state absorption and triplet–triplet absorption of <i>meso</i> -tetra-	253 (2000) 351
phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
An experimental and theoretical study of the valence shell photoelectron spectrum of	,
the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P.	
Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	0.5.4 .00000 .00.5
Niessen Supersonic jet and solution studies of intramolecular complexes with TICT formation	254 (2000) 385
mimicking solute–solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	
and B. Brutschy	254 (2000) 407
Kinetic modelling of radiative reacting gas flow under strong nonequilibrium	
conditions, E.V. Kustova and A. Chikhaoui	255 (2000) 59

)1

Photophysical properties of tris-acetylpyrene derivative of a cryptand in different	
environments, P. Bandyopadhyay, P.K. Bharadwaj, M. Basu Roy, R. Dutta and S.	
Ghosh	255 (2000) 325
Solvent dependence of the intersystem crossing kinetics of thioxanthone, C. Ley, F. Morlet-Savary, P. Jacques and J.P. Fouassier Dipole (e,e+ion) coincidence studies of the ionic photofragmentation and photoioniza-	255 (2000) 335
tion of carbonyl sulfide in the valence shell and S 2p, 2s and C 1s inner shell regions (10–300 eV), R. Feng, G. Cooper, Y. Sakai and C.E. Brion	255 (2000) 353
Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stampor Conical intersections induced by repulsive ${}^{1}\pi\sigma^{\circ}$ states in planar organic molecules:	256 (2000) 351
malonaldehyde, pyrrole and chlorobenzene as photochemical model systems, A.L. Sobolewski and W. Domcke	259 (2000) 181
Femtosecond secondary emission arising from the nonadiabatic photoisomerization in rhodopsin, S. Hahn and G. Stock	259 (2000) 297
Temperature dependent photoabsorption cross sections of allene and methylacetylene in the VUV-UV region, F.Z. Chen, D.L. Judge and C.Y.R. Wu Photoionization studies of C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D.	260 (2000) 215
Scott, F.H. Watson and G.L. Findley UV, VUV and soft X-ray photoabsorption of dimethyl ether by dipole (e,e)	260 (2000) 225
spectroscopies, R. Feng, G. Cooper and C.E. Brion	260 (2000) 391
Photochemistry District the state of the st	
Photodesorption of NO from a metal surface: quantum dynamical implications of a two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce Effect of collisions on the orientational relaxation of photofragments, A.P. Blokhin and	251 (2000) 51
M.F. Gelin	252 (2000) 323
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	
North Photophysical properties of tris-acetylpyrene derivative of a cryptand in different environments, P. Bandyopadhyay, P.K. Bharadwaj, M. Basu Roy, R. Dutta and S.	254 (2000) 309
Ghosh	255 (2000) 325
Photodissociation spectroscopy of ClCN in the vacuum ultraviolet region, K. Kanda, M. Kono, T. Nagata, A. Hiraya, K. Tabayashi and K. Shobatake Light intensity dependence of a two-photon catalytic cycle: photoionization via	255 (2000) 369
absorption-electron transfer-absorption, M. Goez and V. Zubarev	256 (2000) 107
Laser flash photolysis of IrCl ₆ ²⁻ in aqueous solutions, E.M. Glebov, V.F. Plyusnin, N.V. Tkachenko and H. Lemmetyinen	257 (2000) 79
Photodynamics of ethylene: ab initio studies of conical intersections, M. Ben-Nun and T.J. Martínez	259 (2000) 237
Conical intersections in molecular photochemistry – the role of phase change, S. Zilberg and Y. Haas	259 (2000) 249
Control intermedian and abstraction Corr 11 C B	
Conical intersections and photoreactions of 2 <i>H</i> -azirines, C. Bornemann and M. Klessinger Femtosecond secondary emission arising from the nonadiabatic photoisomerization in	259 (2000) 263

253 (2000) 91

Conical intersections, pseudorotation and coherent oscillations in ultrafast photodissociation of group-6 metal hexacarbonyls, S.A. Trushin, W. Fuß and W.E. Schmid	259 (2000) 313
Dihydroazulene/vinylheptafulvene photochromism: dynamics of the photochemical ring-opening reaction, J. Ern, M. Petermann, T. Mrozek, J. Daub, K. Kuldová and	050 (0000) 001
C. Kryschi Substituent effects on the intramolecular proton transfer in the ground and lowest-lying	259 (2000) 331
singlet excited states of salicylaldimine, M. Forés, M. Duran and M. Solà Photodissociation dynamics of CH ₂ BrCl at 234 nm, SH. Lee, YJ. Jung and KH.	260 (2000) 53
Jung	260 (2000) 143
The predissociation dynamics of vibrational eigenstates in the A ² Σ ⁺ state of HBr ⁺ ions: numerical solution of coupled time-dependent Schrödinger equations, M.V. Korolkov and KM. Weitzel	252 (2000) 209
Dielectric relaxation and molecular conformational energy of some arylazo bzen- zothiazine derivatives, M. Kozłowski, H.A. Kołodziej, R. Wieczorek, Z. Latajka and	232 (2000) 209
A. Jurlewicz	252 (2000) 289
The solvent influence on the electrochemical transfer of divalent ions, O. Pecina and W. Schmickler	252 (2000) 349
Energy dissipation and relaxation processes in deoxy myoglobin after photoexcitation	232 (2000) 349
in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochstrasser Quantum and semiclassical dynamics of the Franck-Condon wave packet on the	259 (2000) 71
coupled potential surfaces of the $\widetilde{X}^2A'/\widetilde{A}^2A'$ conical intersection, F . Santoro, C . Petrongolo, G . Granucci and M . Persico	259 (2000) 193
A model study of the wavepacket dynamics around a Jahn–Teller conical intersection in	257 (2000) 175
a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani	259 (2000) 201
Intramolecular dynamics	
Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy, N. Došlić and O. Kühn	255 (2000) 247
Solvent dependence of the intersystem crossing kinetics of thioxanthone, C. Ley, F.	
Morlet-Savary, P. Jacques and J.P. Fouassier Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P.	255 (2000) 335
Plaza, W. Rettig and M.M. Martin	256 (2000) 137
Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic B State, A. Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H.	(,
Baumgärtel	256 (2000) 239
Energy dissipation and relaxation processes in deoxy myoglobin after photoexcitation in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochstrasser	259 (2000) 71
Quantum and semiclassical dynamics of the Franck-Condon wave packet on the coupled potential surfaces of the $\widetilde{X}^2A'/\widetilde{A}^2A'$ conical intersection, F. Santoro, C.	239 (2000) 71
Petrongolo, G. Granucci and M. Persico	259 (2000) 193
A model study of the wavepacket dynamics around a Jahn-Teller conical intersection in a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani	259 (2000) 201
-radiationless transitions	
Excited-state intramolecular proton transfer followed by <i>cis-trans</i> isomerization of (1-	
hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and	
LI Chizuka	252 (2000) 01

1 07

H. Shizuka

Relaxation of individual rotational levels of the \tilde{A}^1Au electronic state of acetylene	
excited to the $2v_3'$ and $(v_1' + v_3' + v_6')$ vibrational modes, V.I. Makarov and E.	253 (2000) 259
Quiñones Optical transitions from the chlorine $O_{\mu}^{+}(^{3}P_{2})$ ion-pair state, N.K. Bibinov, A.A. Fateev,	233 (2000) 239
D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
-vibrational energy redistribution (incl. vibrational dissociation)	
The predissociation dynamics of vibrational eigenstates in the $A^2\Sigma^+$ state of HBr ⁺ ions: numerical solution of coupled time-dependent Schrödinger equations, M.V.	252 (2000) 200
Korolkov and KM. Weitzel A classical algebraic approach to the bend motion of acetylene: the formalism by two	252 (2000) 209
coupled cosets, G. Wu Observation of a bottleneck in the vibrational relaxation of liquid bromoform,	252 (2000) 315
M.A.F.H. van den Broek and H.J. Bakker Impulsive IR-multiphoton dissociation of acrolein: observation of non-statistical product vibrational excitation in CO ($v = 1-12$) by time resolved IR fluorescence	253 (2000) 157
spectroscopy, P.K. Chowdhury	260 (2000) 151
Vibrational energy storage in high pressure mixtures of diatomic molecules, E. Plönjes, P. Palm, W. Lee, M. D. Chidley, I.V. Adamovich, W. R. Lempert and J.W. Rich	260 (2000) 353
Luminescence spectra, yields and lifetimes	
Magnetic fluorescence quenching of the NO β(0-9) transition, V.I. Makarov, I.V. Khmelinskii, S.A. Kochubei and V.N. Ishchenko	252 (2000) 379
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek Photodissociation spectroscopy of ClCN in the vacuum ultraviolet region, K. Kanda,	254 (2000) 319
M. Kono, T. Nagata, A. Hiraya, K. Tabayashi and K. Shobatake Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclote-	255 (2000) 369
tradecane)chromium(III) nitrate, JH. Choi Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate	256 (2000) 29
methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A.	
Costela, I. García-Moreno, R. Sastre and F.J. Duarte Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for	256 (2000) 125
organic light-emitting diodes, W. Stampor Optical spectroscopy and crystal-field effects on the paramagnetic susceptibility of rare-earth germanates $GaRGe_2O_7$, $R = Pr$, Nd, C. Cascales, G. Lozano, C. Zaldo and P.	256 (2000) 351
Porcher	257 (2000) 29
Effect of solvent polarizability on dual fluorescence of <i>EE</i> -1-phenyl,4-(1'-pyrenyl)-1,3-butadiene, E. Marri, G. Galiazzo, U. Mazzucato and A. Spalletti	260 (2000) 383
Coherence loss processes	
Quasi-particle lifetimes on noble metal surfaces studied by ARPES and STM, R. Matzdorf	251 (2000) 151
Quantum beats in recombination of spin-correlated radical ion pairs with equivalent protons, V.A. Bagryansky, O.M. Usov, V.I. Borovkov, T.V. Kobzeva and Yu.N.	
Molin	255 (2000) 237

)9

,	12
Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli	256 (2000) 265
Nonlinear responses (incl. optical)	
Surface collective excitations in ultrafast pump-probe spectroscopy of metal nanopar-	
ticles, T.V. Shahbazyan and I.E. Perakis	251 (2000) 37
Electron dynamics in metallic nanoparticles, JY. Bigot, V. Halté, JC. Merle and A.	
Daunois	251 (2000) 181
Electron dynamics and surface plasmon resonance nonlinearities in metal nanoparti-	
cles, N. Del Fatti, F. Vallée, C. Flytzanis, Y. Hamanaka and A. Nakamura	251 (2000) 215
Electron and lattice dynamics following optical excitation of metals, J. Hohlfeld, SS.	
Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias	251 (2000) 237
Ultrafast optical relaxation dynamics in metallic nanoparticles: from bulk-like toward spatial confinement regime, S. Stagira, M. Nisoli, S. De Silvestri, A. Stella, P.	
Tognini, P. Cheyssac and R. Kofman	251 (2000) 259
Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic	251 (2000) 200
generation, YM. Chang, L. Xu and H.W.K. Tom	251 (2000) 283
Coherence control of currents in semiconductors: a materials perspective, H.M. van Driel	251 (2000) 200
Zwitterionic polymers for nonlinear optics, C. Combellas, F. Kajzar, G. Mathey, M.A.	251 (2000) 309
Petit and A. Thiébault	252 (2000) 165
An improved calculation method on optical second-order susceptibilities of organic	232 (2000) 103
materials, XL. Zhu, XZ. You, Y. Zhong, Z. Yu and SL. Guo	253 (2000) 241
Channels of the exciton–exciton annihilation in one-dimensional aggregates at low	255 (2000) 241
temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
A novel approach to calculation of the second-order nonlinear optical susceptibilities of	20. (2000) 51
organic crystals based on energy-band theory, XL. Zhu, XZ. You and Y. Zhang	254 (2000) 287
Prediction of pure electric-dipole two-photon absorption circular dichroism in	(
lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach	
toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J.	
Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
Optimization of the molecular hyperpolarizability for second harmonic generation in	
chiral media, V. Ostroverkhov, O. Ostroverkhova, R.G. Petschek, K.D. Singer, L.	
Sukhomlinova, R.J. Twieg, SX. Wang and L.C. Chien	257 (2000) 263
Vibrational corrections to linear and nonlinear static electric properties of polyatomic	
molecules at non-optimum reference geometry, V.E. Ingamells, M.G. Papadopoulos	
and A.J. Sadlej	260 (2000) 1
Multiphoton phenomena	
Electron–photon field dynamics: numerically exact calculations of multi-state molecule	
systems interacting with a single-mode coherent photon field, M. Nakano and K.	
Yamaguchi	252 (2000) 115
	202 (2000) 113
Desired to the transfer of	
Reactions (incl. dissociation) The attractive quartet potential approxy surface for the GU C(c4A) CO reaction H	
The attractive quartet potential energy surface for the CH ₃ C(a ⁴ A ₂) + CO reaction, H. Hou, B. Wang and Y. Gu	252 (2000) 17
Hou, b. wang and 1. Ou	252 (2000) 17

A genetic algorithm based technique for locating first-order saddle point using a	
gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp	253 (2000) 295
Temperature dependence of fast neutral-neutral reactions: a triatomic model study, A.	
Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	
CO ₂ + H ₂ → HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud- Dandine and A. Sevin	254 (2000) 00
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR	254 (2000) 99
matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
A theoretical study on a Diels-Alder reaction in ambient and supercritical water:	254 (2000) 201
viewing solvent effects through frontier orbitals, Y. Harano, H. Sato and F. Hirata	258 (2000) 151
Ab initio study of the reaction mechanism of singlet and triplet N ₂ O and their	
intersystem crossing, DY. Hwang and A.M. Mebel	259 (2000) 89
The geometric phase effect in chemical reactions, S. Adhikari and G.D. Billing	259 (2000) 149
Conical intersections in molecular photochemistry - the role of phase change, S. Zilberg	
and Y. Haas	259 (2000) 249
Conical intersections, pseudorotation and coherent oscillations in ultrafast photo-	
dissociation of group-6 metal hexacarbonyls, S.A. Trushin, W. Fuß and W.E.	
Schmid	259 (2000) 313
Recombination yield of geminate radical pairs in high magnetic fields: general results	260 (2000) 125
and application to free diffusion, M.J. Hansen, A.A. Neufeld and J.B. Pedersen Photoionization mass spectrometry of six isomers of C ₇ H ₈ in the 7–22 eV photon	260 (2000) 125
energy range, M. Schwell, F.v. Dulieu, C. Gée, HW. Jochims, JL. Chotin, H.	
Baumgreel and S. Leach	260 (2000) 261
Linear and convolution methods for the analysis of ground and excited state kinetics.	200 (2000) 201
Application to the monomer–excimer scheme, M.N. Berberan-Santos, J.P.S. Farinha	
and J.M.G. Martinho	260 (2000) 401
-isolated molecules	
The predissociation dynamics of vibrational eigenstates in the $A^2\Sigma^+$ state of HBr ⁺ ions:	
numerical solution of coupled time-dependent Schrödinger equations, M.V.	
Korolkov and KM. Weitzel	252 (2000) 209
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination	
channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	
North	254 (2000) 309
Photomobility of O(¹ D) atom in solid Ar and its reaction with CF ₃ I, M. Chen, X.	
Wang, L. Zhang, Q. Qin and Q. Zheng	255 (2000) 95
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, DY. Hwang and A.M. Mebel	256 (2000) 160
Photodissociation dynamics of CH ₂ BrCl at 234 nm, SH. Lee, YJ. Jung and KH.	256 (2000) 169
Jung	260 (2000) 143
	200 (2000) 143
-collisional	
Time-dependent quantum dynamics study of reactive scattering of the HD + CN system	
in the potential averaged 5D model, Y. Zhang, Z. Tan, H. Zhang, Q. Zhang and	
J.Z.H. Zhang	252 (2000) 191

Study of electron polarization and correlation effects in resonant and background		
electron scattering off CF ₃ Cl, T. Beyer, B.M. Nestmann and S.D. Peyerimhoff Quasiclassical calculation of the chemical reaction Sr + HF, MQ. Cai, L. Zhang, BY.	255 (2000)	1
Tang, MD. Chen, GW. Yang and KL. Han Reactant-product decoupling approach to state-to-state reactive scattering H+DH, S.	255 (2000) 2	83
Zhang, Z. Tan, H. Zhang, Y. Zhang and J.Z.H. Zhang	255 (2000) 3	197
State selected reactions of krypton ions with methane, A. Kok, P.A.Z. van Emmichoven and A. Niehaus	258 (2000)	47
Production processes of H(D) atoms in the reactions of NO($A^2\Sigma^+$) with C_2H_2 , C_2H_4 , H_2O , and their isotopic variants, H. Umemoto, N. Terada, K. Tanaka, T.	200 (2000)	
Takayanagi, Y. Kurosaki and K. Yokoyama Quasi-classical trajectory simulations of C + NO crossed molecular beam experiments,	259 (2000)	39
S. Andersson, N. Marković and G. Nyman	259 (2000)	99
-condensed phase		
Calculation of CIDNP field dependences in biradicals in the photolysis of large-ring cycloalkanones, A.V. Popov, P.A. Purtov and A.V. Yurkovskaya	252 (2000)	02
Temperature-independent onset of diffusion control during polymerization in a diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A.	252 (2000)	0.3
Wasylyshyn and G.P. Johari Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	252 (2000)	237
charge transfer reactions in solution, A. Samanta and S.K. Ghosh Kinetic energy distributions for O ⁻ and metastable CO [*] produced by electron	254 (2000)	39
stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y.L. Coat, P. Cloutier and L. Sanche	254 (2000)	69
High resolution near infrared spectrum of solid nitrogen, pure and doped with carbon dioxide, F. Legay and N. Legay-Sommaire	257 (2000)	103
Solvent effect on Sr ²⁺ to Ca ²⁺ ion mutation: Monte Carlo simulation study, HS. Kim	257 (2000)	
Liquid water ionization: mechanistic implications of the H/D isotope effect in the geminate recombination of hydrated electrons, M.U. Sander, M.S. Gudiksen, K.		
Luther and J. Troe	258 (2000)	257
Extent of inter-hydrogen bond correlations in water. Temperature effect, A. Luzar	258 (2000)	267
Tunneling Tunneling enlittings in vibrational enestre of non-rigid melacules V.A. Banderskii and		
Tunneling splittings in vibrational spectra of non-rigid molecules, V.A. Benderskii and E.V. Vetoshkin	257 (2000)	203
The anomalous Stark effect of single terrylene molecules in <i>p</i> -terphenyl crystals, P. Bordat, M. Orrit, R. Brown and A. Würger	258 (2000)	63
Electron transfer		
Influence of Xe adlayer morphology and electronic structure on image-potential state lifetimes of Ru(0001), W. Berthold, U. Höfer, P. Feulner and D. Menzel	251 (2000)	123
Ultrafast electron dynamics at surfaces probed by resonant Auger spectroscopy, W. Wurth and D. Menzel	251 (2000)	141
Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems:	252 (2020)	212
ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp	253 (2000)	313

)9

Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W.	
Rettig	253 (2000) 339
Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras- Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat Vibronic model of hyperfine interaction in dimeric mixed-valence clusters, A.V. Palii,	254 (2000) 275
M.I. Belinsky and B.S. Tsukerblat	255 (2000) 51
Photophysical properties of tris-acetylpyrene derivative of a cryptand in different environments, P. Bandyopadhyay, P.K. Bharadwaj, M. Basu Roy, R. Dutta and S. Ghosh	255 (2000) 325
Light intensity dependence of a two-photon catalytic cycle: photoionization via	200 (2000) 220
absorption-electron transfer-absorption, M. Goez and V. Zubarev Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P.	256 (2000) 107
Plaza, W. Rettig and M.M. Martin	256 (2000) 137
Isomerism of the covalent anion of the dimer of uracil and 1-methyl-cytosine: ab initio study, I. Al-Jihad, J. Smets and L. Adamowicz	257 (2000) 167
Quantum dynamics of model proton-coupled electron transfer reactions, S. Shin and SI. Cho	259 (2000) 27
A model study of the wavepacket dynamics around a Jahn-Teller conical intersection in a symmetric charge-transfer system, A. Ferretti, A. Lami and G. Villani Ab initio calculation for inner reorganization energy of gas-phase electron transfer in	259 (2000) 201
organic molecule-ion systems, XY. Li, J. Tong and FC. He	260 (2000) 283
Proton and hydrogen atom transfer	
Protonation of archetypal aromatic and antiaromatic systems - G2 studies of benzene	
and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar Excited-state intramolecular proton transfer followed by <i>cis-trans</i> isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and	
H. Shizuka	253 (2000) 91
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Monitoring laser driven hydrogen atom motion by transient infrared spectroscopy, N. Došlić and O. Kühn	255 (2000) 247
Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y.	
Gauduel and H. Gelabert	256 (2000) 333
Computation of the pK of liquid water using coordination constraints, M. Sprik A multi-state empirical valence bond model for acid-base chemistry in aqueous	258 (2000) 139
solution, M. uma, U.W. Schmitt and G.A. Voth Quantum dynamics of model proton-coupled electron transfer reactions, S. Shin and	258 (2000) 187
SI. Cho	259 (2000) 27
Substituent effects on the intramolecular proton transfer in the ground and lowest-lying	g
singlet excited states of salicylaldimine, M. Forés, M. Duran and M. Solà	260 (2000) 53
Positron annihilation	
Pressure quenching of positronium in solid biphenyl, T. Goworek, T. Suzuki, E Hamada, K. Kondo and Y. Ito	255 (2000) 347

Luther and J. Troe

258 (2000) 257

Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre	255 (2000) 207
and I. Billard	256 (2000) 307
Ionization (incl. Rydberg states)	
Energy dependences of fragment ion yields from acetone photoexcited in the C1s and	
Ols transition regions, I.H. Suzuki and N. Saito	253 (2000) 351
Dispersive photoelectron spectroscopy of the ungerade Rydberg states of Xe ₂ near	
Xe*(6p,5d), D.M. Mao, X.K. Hu, Y.J. Shi and R.H. Lipson	257 (2000) 253
About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine	
structure and its vibrational analysis, R. Locht, B. Leyh, A. Hoxha, D. Dehareng, H.W. Jochims and H. Baumgärtel	257 (2000) 202
Analysis of the bound odd-parity spectrum of krypton by weakest bound electron	257 (2000) 283
potential model theory, N.W. Zheng, T. Zhou, R. Yang, T. Wang and D. Ma	258 (2000) 37
Liquid water ionization: mechanistic implications of the H/D isotope effect in the	250 (2000) 57
geminate recombination of hydrated electrons, M.U. Sander, M.S. Gudiksen, K.	
Luther and J. Troe	258 (2000) 257
Photoionization studies of C ₂ H ₅ I and C ₆ H ₆ perturbed by Ar and SF ₆ , C.M. Evans, J.D.	
Scott, F.H. Watson and G.L. Findley	260 (2000) 225
The photoabsorption and constant ionic state spectroscopy of vinylbromide, A. Hoxha,	260 (2000) 207
R. Locht, B. Leyh, D. Dehareng, K. Hottmann, H.W. Jochims and H. Baumgrtel	260 (2000) 237
Vertical triple ionization of ethyne molecules in triple-electron-transfer collisions with O ²⁺ beam ions, N. Jeffreys, D.E. Parry and F.M. Harris	260 (2000) 295
o beam ions, iv. Jenicys, D.E. Farry and F.M. Harris	200 (2000) 293
Molecular motion (incl. diffusive)	
Motional effects on optimum coherence transfer in ² H MAS NMR spectroscopy, J.H.	
Kristensen, G.L. Hoatson and R.L. Vold	252 (2000) 97
Molecular motions in molecular glasses as studied by thermally stimulated depolarisa-	
tion currents (TSDC), N.T. Correia, C. Alvarez, J.J. Moura Ramos and M.	
Descamps	252 (2000) 151
Self-diffusion in liquid metals, A.S. Chauhan, R. Ravi and R.P. Chhabra	252 (2000) 227
Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martín Negri and P.F. Aramendía	253 (2000) 249
Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave	255 (2000) 249
number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa,	
C. Abematsu, S. Yajima and K. Ishii	253 (2000) 331
Photomobility of O(¹ D) atom in solid Ar and its reaction with CF ₃ I, M. Chen, X.	222 (2000) 001
Wang, L. Zhang, Q. Qin and Q. Zheng	255 (2000) 95
Dielectric relaxations of collagen and elastin in the dehydrated state, V. Samouillan, A.	
Lamure and C. Lacabanne	255 (2000) 259
Relaxational dynamics of water molecules at protein surface, S. Dellerue and MC.	0.50 (0.000) 4:5
Bellissent-Funel	258 (2000) 315
Isotopic effects	
Liquid water ionization: mechanistic implications of the H/D isotope effect in the	
geminate recombination of hydrated electrons, M.U. Sander, M.S. Gudiksen, K.	
Luther and I Tree	258 (2000) 257

Production processes of $H(D)$ atoms in the reactions of $NO(A^2\Sigma^+)$ with C_2H_2 , C_2H_4 , H_2O , and their isotopic variants, H . Umemoto, N . Terada, K . Tanaka, T . Takayanagi, Y . Kurosaki and K . Yokoyama	259 (2000) 39
Fluctuations and noise Stretched exponentials and barrier distributions, O. Edholm and C. Blomberg	252 (2000) 221
Collective motion and excitations Electron dynamics in metallic nanoparticles, JY. Bigot, V. Halte, JC. Merle and A. Daunois Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii Mandelstam-Brillouin spectra and hyperacoustic velocities dispersion of trideutero-acetonitrile in the liquid state, R.S. Cataliotti, P. Sassi, A. Morresi and G. Paliani	251 (2000) 181 253 (2000) 331 255 (2000) 85
 Surface chemical physics Photodesorption of NO from a metal surface: quantum dynamical implications of a two-mode model, P. Saalfrank, G. Boendgen, K. Finger and L. Pesce Hot-electron femtochemistry at surfaces: on the role of multiple electron processes in desorption, J.W. Gadzuk Ultrafast transient grating scattering studies of carrier dynamics at a silicon surface, T. Sjodin, CM. Li, H. Petek and HL. Dai Coherent phonon spectroscopy of GaAs surfaces using time-resolved second-harmonic generation, YM. Chang, L. Xu and H.W.K. Tom Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini The self-diffusivity of amorphous solid water near 150 K, R.S. Smith, Z. Dohnálek, G.A. Kimmel, K.P. Stevenson and B.D. Kay A theoretical analysis of the sum frequency generation spectrum of the water surface, A. Morita and J.T. Hynes 	251 (2000) 51 251 (2000) 87 251 (2000) 205 251 (2000) 283 253 (2000) 367 258 (2000) 291 258 (2000) 371
 -surface scattering Dynamical Lie algebraic approach to rotationally inelastic scattering of molecules from surfaces, D. Guan, X. Yi, Y. Zheng, S. Ding and J. Sun Statistical dynamics in rotationally inelastic gas-surface scattering: dynamical Lie algebraic method, Y. Zheng, X. Yi, D. Guan and Q. Meng 	252 (2000) 179 255 (2000) 273
-adsorption Femtosecond two-photon photoemission studies of image-potential states, T. Fauster, C. Reuß, I.L. Shumay and M. Weinelt Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin	251 (2000) 111 253 (2000) 367 256 (2000) 61

-desorption Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to	
catalytic processes, E. Molinari and M. Tomellini Kinetic energy distributions for O ⁻ and metastable CO [*] produced by electron	253 (2000) 367
stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y.L. Coat, P. Cloutier and L. Sanche Fine level splitting of aggregate neodymium centers in CaF ₂ crystals, V.V. Fedorov, W.	254 (2000) 69
Beck, T.T. Basiev, A.Ya. Karasik and C. Flytzanis	257 (2000) 275
-surface excitations	
The role of Auger decay in hot electron excitation in copper, H. Petek, H. Nagano, M.J. Weida and S. Ogawa	251 (2000) 71
Femtosecond electron dynamics at the benzene/Ag(111) interface, K.J. Gaffney, C.M.	251 (2000) 71
Wong, S.H. Liu, A.D. Miller, J.D. McNeill and C.B. Harris Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to	251 (2000) 99
catalytic processes, E. Molinari and M. Tomellini	253 (2000) 367
-adsorbate structure	
Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer	256 (2000) 37
-catalysis	
Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini	253 (2000) 367
Electronic process in gases	
The effect of carbonyl complexation on highly exothermic vanadium oxidation	260 (2000) 267
reactions, M.J. McQuaid and J.L. Gole	260 (2000) 367
Thermodynamic and transport properties	
Electron and lattice dynamics following optical excitation of metals, J. Hohlfeld, SS. Wellershoff, J. Güdde, U. Conrad, V. Jähnke and E. Matthias Nuclear quadrupole coupling constant of ²¹ Ne in the neon dimer and its influence on	251 (2000) 237
the T_1 NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and M. Jaszuński	253 (2000) 183
Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón	255 (2000) 73
Influence of the local electric field on ionic transport during redox switching of	255 (2000) 201
conducting polymers, F. Miomandre, M.N. Bussac, E. Vieil and L. Zuppiroli Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-	255 (2000) 291
methylcyclopentanone, D. Kim and T. Baer	256 (2000) 251
The isotopic and temperature dependent properties of hydrogen chloride dissolved in carbon tetrachloride. A molecular dynamics approach, G. Chatzis and J. Samios	257 (2000) 51

Structure of solids, liquids and glasses Ultrafast electron and lattice dynamics in semiconductors at high excited carrier densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur Temperature-independent onset of diffusion control during polymerization in a diepoxide-amine mixture by dielectric measurements, J.G. McAnanama, D.A. Wasylsyshyn and G.P. Johari The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman Monte Carlo simulation study of solvent effect on Na* to Li* ion mutation, HS. Kim Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an a	The self-diffusivity of amorphous solid water near 150 K, R.S. Smith, Z. Dohnálek, G.A. Kimmel, K.P. Stevenson and B.D. Kay Slow dynamics in supercooled water, F. Sciortino	258 (2000) 291 258 (2000) 307
The structure of liquid clusters of Lennard-Jones atoms, B.G. Moore and A.A. Al-Quraishi Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman Monte Carlo simulation study of solvent effect on Na* to Li* ion mutation, HS. Kim Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H··O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Ba Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and	Ultrafast electron and lattice dynamics in semiconductors at high excited carrier densities, J.P. Callan, A.MT. Kim, L. Huang and E. Mazur Temperature-independent onset of diffusion control during polymerization in a	251 (2000) 167
Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman Monte Carlo simulation study of solvent effect on Na* to Li* ion mutation, HS. Kim Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323 Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani 254 (2000) 215 Thermodynamic, structural, and dynamic study of the N-HO=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón 255 (2000) 73 The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully 258 (2000) 427 (250 (2000) 183 (251 (2000) 227 (250 (2000) 337 (250 (2000		252 (2000) 237
Monte Carlo simulation study of solvent effect on Na* to Li* ion mutation, HS. Kim Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H··O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 45°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Quraishi	252 (2000) 337
Monte Carlo simulation study of solvent effect on Na* to Li* ion mutation, HS. Kim Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H··O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 45°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman	253 (2000) 267
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Monte Carlo simulation study of solvent effect on Na ⁺ to Li ⁺ ion mutation, HS. Kim	
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted	
Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen—water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		253 (2000) 323
Paesani Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen—water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Structural properties and quantum effects in protonated helium clusters. II. Quantum	
Thermodynamic, structural, and dynamic study of the N-H···O=C hydrogen bond association in aqueous solution, S. Tolosa, A. Hidalgo and J.A. Sansón The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettit Nature of collagen—water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		254 (2000) 215
The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation, A.A. Chialvo, E. Yezdimer, T. Driesner, P.T. Cummings and J.M. Simonson Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettit Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		
Solvation structures in three dimensions, I.M. Svishchev, A.Yu. Zassetsky and P.G. Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen—water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	The structure of water from 25°C to 457°C: comparison between neutron scattering and	
Kusalik Semi-grand canonical molecular dynamics simulation of bovine pancreatic trypsin inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen—water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	J.M. Simonson	258 (2000) 109
inhibitor, G.C. Lynch and B.M. Pettitt Nature of collagen-water hydration forces: a problem in water structure, G.E. Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		258 (2000) 181
Walrafen and YC. Chu A rigorous procedure for combining molecular dynamics and Monte Carlo simulation algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		258 (2000) 405
algorithms, L.J. LaBerge and J.C. Tully Critical behavior and phase transitions Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		258 (2000) 427
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		260 (2000) 183
Laser induced dynamic spectral weight transfer in La _{0.7} Ca _{0.3} MnO ₃ , A.I. Lobad, A.J. Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		
Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell Effect of hydrostatic pressure on phase transitions in spin-crossover 1D systems, S. Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		
Klokishner, J. Linares and F. Varret Low-temperature elastic anomalies in an anthracene single crystal, M. Fukuhara, A.H. Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Taylor, C. Kwon, S.A. Trugman and T.R. Gosnell	251 (2000) 227
Matsui and M. Takeshima A modified perturbed hard-sphere-chain equation of state: consideration of attractive contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,	Klokishner, J. Linares and F. Varret	255 (2000) 317
contribution, I.H. Kim and Y.C. Bae Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		258 (2000) 97
adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco 256 (2000) 259 Molecular self-assembly and -organization Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		260 (2000) 337
Coupling of diffusion and reaction in the process of capillary formation in alginate gel,		256 (2000) 259
		252 (2000) 199

Structure-function self-organization in nonequilibrium macromolecular systems. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik	, L.N. 256 (2000) 45
Biomolecular structure-function relationships	
The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical	study
using combined discrete/self-consistent reaction field models, C. Alemán	253 (2000) 13
Structure-function self-organization in nonequilibrium macromolecular systems	, L.N.
Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik	256 (2000) 45
Semi-grand canonical molecular dynamics simulation of bovine pancreatic t	rypsin
inhibitor, G.C. Lynch and B.M. Pettitt	258 (2000) 405
Hydration structure of the α-chymotrypsin substrate binding pocket: the imp	3 4
constrained geometry, C. Carey, YK. Cheng and P.J. Rossky	258 (2000) 415
Energy dissipation and relaxation processes in deoxy myoglobin after photoexci	
in the Soret region, Y. Kholodenko, M. Volk, E. Gooding and R.M. Hochst	
, , , , , , , , , , , , , , , , , , , ,	()



(continued from inside front cover)

Submission of papers: All papers should be submitted in quadruplicate to one of the editors.

Electronic manuscripts: Electronic manuscripts have the advantage that there is no need for the rekeying of text, thereby avoiding the possibility of introducing errors and resulting in reliable and fast delivery of proofs.

For the initial submission of manuscripts for consideration, hardcopies are sufficient. For the processing of accepted papers, electronic versions are preferred. After final acceptance, your disk plus one final and exactly matching printed version should be submitted together. Double density (DD) or high density (HD) diskettes (3.5 or 5.25 inch) are acceptable. It is important that the file saved is in the native format of the wordprocessor program used. Label the disk with the name of the computer and wordprocessing package used, your name, and the name of the file on the disk.

Important: please adhere to instructions to authors, to be found on the last pages of each volume. The instructions can also be found on the World Wide Web: access under http://www.elsevier.nl or http://www.elsevier.com.

Proofs and reprints: Authors will receive proofs, which they are requested to correct and return as soon as possible. No new material may be inserted in the text at the time of proofreading. A total of 50 reprints of each paper will be supplied free of charge to the author(s). Additional reprints can be ordered at prices shown on the reprint order form,

All questions arising after acceptance of the manuscript, especially those relating to proofs, should be directed to Chemical Physics, Elsevier Science B.V., P.O. Box 2759, 1000 CT Amsterdam, The Netherlands. Tel. (+31-20)4852-800, Fax (+31-20)4852-775, E-mail: e.hovens@elsevier.nl

Authors in Japan please note: Upon request, Elsevier Science K.K. will provide authors with a list of people who can check and improve the English of their paper (before submission). Please contact our Tokyo office: Elsevier Science K.K., 9-15 Highashi-Azabu 1-chome Minato-ku, Tokyo 106-0044, Tel. (03)-5561-5032; Fax (03)-5561-5045.

Chemical Physics has no page charges.

Publication Information: Chemical Physics (ISSN 0301-0104) For 2000, volumes 252-263 are scheduled for publication. Subscription prices are available upon request from the Publisher or from the Regional Sales Office nearest you or from this journal's website (http://www.elsevier.nl/locate/chemphys). Further information is available on this journal and other Elsevier Science products through Elsevier's website: http://www.elsevier.nl. Subscriptions are accepted on a prepaid basis only and are entered on a calendar year basis. Issues are sent by standard mail (surface within Europe, air delivery outside Europe). Priority rates are available upon request. Claims for missing issues should be made within six months of the date of dispatch.

Orders, claims, and product enquiries: please contact the Customer Support Department at the Regional Sales Office nearest you:

New York: Elsevier Science, P.O. Box 945, New York, NY 10159-0945, USA; phone: (+1) (212) 633-3730 [toll free number for North American customers: 1-888-4ES-INFO (437-4636)]; fax: (+1) (212) 633-3680; e-mail: usinfo-f@elsevier.com

Amsterdam: Elsevier Science, P.O. Box 211, 1000 AE Amsterdam, The Netherlands; phone: (+31) 20 4853757; fax: (+31) 20 4853432; e-mail: nlinfo-f@elsevier.nl

Tokyo: Elsevier Science, 9-15 Higashi-Azabu 1-chome, Minato-ku, Tokyo 106-0044, Japan; phone: (+81) (3) 5561 5033; fax: (+81) (3) 5561 5047; e-mail: info@elsevier.co.jp

Singapore: Elsevier Science, No. 1 Temasek Avenue, #17-01 Millenia Tower, Singapore 039192; phone: (+65) 434 3727; fax: (+65) 337 2230; e-mail: asiainfo@elsevier.com.sg

Rio de Janeiro: Elsevier Science, Rua Sete de Setembro 111/16 Andar, 20050-002 Centro, Rio de Janeiro - RJ, Brazil; phone: (+55) (21) 509 5340; fax: (+55) (21) 507 1991; e-mail: elsevier@campus.com.br [Note (Latin America): for orders, claims and help desk information, please contact the Regional Sales Office in New York as listed above]

Advertising information. Advertising orders and enquiries can be sent to: USA, Canada and South America: Mr Tino de Carlo, The Advertising Department, Elsevier Science Inc., 655 Avenue of the Americas, New York, NY 10010-5107, USA; phone: (+1) (212) 633 3815; fax: (+1) (212) 633 3820; e-mail: t.decarlo@elsevier.com. Japan: The Advertising Department, Elsevier Science K.K., 9-15 Higashi-Azabu 1chome, Minato-ku, Tokyo 106-0044, Japan; phone: (+81) (3) 5561-5033; fax: (+81) (3) 5561 5047. Europe and ROW: Rachel Leveson-Gower, The Advertising Department, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK; phone: (+44) (1865) 843565; fax: (+44) (1865) 843976; e-mail: r.leveson-gower@elsevier.co.uk.

US mailing notice: Chemical Physics (ISSN 0301-0104) is published semi-monthly by Elsevier Science B.V. (P.O. Box 211, 1000 AE Amsterdam, The Netherlands). Annual subscription price in the USA US\$5530.00 (valid in North, Central and South America), including air speed delivery. Application to mail at periodical postage rate is paid at Jamaica, NY 11431.

USA POSTMASTER: Send address changes to Chemical Physics, Publications Expediting Inc., 200 Meacham Ave, Elmont, NY 11003.

AIRFREIGHT AND MAILING in the USA by Publications Expediting Inc., 200 Meacham Avenue, Elmont, NY 11003.



The FREE e-mail service which delivers Elsevier Science book and journal tables of contents directly to your PC

Cirect

Sign-up is simple!

- ALL YOU HAVE TO DO IS VISIT THE CONTENTSDIRECT WEBSITE
- POLLOW THE INSTRUCTIONS TO REGISTER YOUR BOOK AND JOURNAL INTERESTS ONLINE
- THEN SIT BACK AND ENJOY
 ADVANCE E-MAIL NOTIFICATION
 OF THE VERY LATEST RESEARCH
 IN YOUR AREAS OF INTEREST

REGISTER TODAY

www.elsevier.com/locate/contentsdirect







